Volume 70B
Number 2
Apr.–June 1966

Mathematics and Mathematical Physics

U.S. DEPARTMENT OF COMMERCE

SECTION B

JOURNAL OF RESEARCH

NATIONAL BUREAU OF STANDARDS

Journal of Research

of the

National Bureau of Standards

B. Mathematics and Mathematical Physics

APR.–JUNE • 1966

VOLUME • 70B

NUMBER • 2

Editor: Chester H. Page

Associate Editor: John J. Sopka

Publication dates: Mar. 10, June 10, Sept. 10, Dec. 10 1966

JOURNAL OF RESEARCH

The National Bureau of Standards Journal of Research reports research and development in the fields of activity shown at right. Also included from time to time are survey articles on topics closely related to the Bureau's scientific and technical program.

The Journal is published in three separate sections as follows:

A. Physics and Chemistry

Contains papers of interest primarily to scientists working in these fields. Issued six times a year. Annual subscription: domestic, $5.00; foreign, $6.00. Single copy $1.00.

B. Mathematics and Mathematical Physics

Presents studies and compilations designed mainly for the mathematician and the theoretical physicist. Issued quarterly. Annual subscription: domestic, $2.25; foreign, $2.75. Single copy 75c.

C. Engineering and Instrumentation

Reports research and development results of interest chiefly to the engineer and the applied scientist. Issued quarterly. Annual subscription: domestic, $2.75; foreign, $3.50. Single copy 75c.

The National Bureau of Standards is a principal focal point in the Federal Government for assuring maximum application of the physical and engineering sciences to the advancement of technology in industry and commerce. Its responsibilities include development and maintenance of the national standards of measurement, and the provisions of means for making measurements consistent with those standards; determination of physical constants and properties of materials; development of methods for testing materials, mechanisms, and structures, and making such tests as may be necessary, particularly for government agencies; cooperation in the establishment of standard practices for incorporation in codes and specifications; advisory service to government agencies on scientific and technical problems; invention and development of devices to serve special needs of the Government; assistance to industry, business and consumers in the development and acceptance of commercial standards and simplified trade practice recommendations; administration of programs in cooperation with United States business groups and standards organizations for the development of international standards of practice; and maintenance of a clearinghouse for the collection and dissemination of scientific, technical, and engineering information. The scope of the Bureau's activities is suggested in the following listing of its three Institutes and their organizational units.

Institute for Basic Standards. Applied Mathematics. Electricity. Metrology. Mechanics. Heat. Atomic Physics. Physical Chemistry. Laboratory Astrophysics.* Radiation Physics. Radio Standards Laboratory:* Radio Standards Physics; Radio Standards Engineering. Office of Standard Reference Data.

Institute for Materials Research. Analytical Chemistry. Polymers. Metallurgy. Inorganic Materials. Reactor Radiations. Cryogenics.* Materials Evaluation Laboratory. Office of Standard Reference Materials.

Institute for Applied Technology. Building Research. Information Technology. Performance Test Development. Electronic Instrumentation. Textile and Apparel Technology Center. Technical Analysis. Office of Weights and Measures. Office of Engineering Standards. Office of Invention and Innovation. Office of Technical Resources. Clearinghouse for Federal Scientific and Technical Information.**

*Located at Boulder, Colorado 80301.
**Located at 5185 Port Royal Road, Springfield, Virginia 22151.

U.S. DEPARTMENT OF COMMERCE
John T. Connor, Secretary
NATIONAL BUREAU OF STANDARDS
A. V. Astin, Director

Order all publications from the Superintendent of Documents
U.S. Government Printing Office, Washington, D.C., 20402.

Use of funds for printing this publication approved by the Director of the Bureau of the Budget (June 22, 1966).

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematics and Mathematical Physics
Vol. 70B, No. 2, April–June 1966

On a Sequence of Points of Interest for Numerical Quadrature

Seymour Haber

Institute for Basic Standards, National Bureau of Standards, Washington, D.C.

(February 15, 1966)

The distribution of 2 sequences of points, originally discussed by van der Corput and by K. F. Roth, is studied in detail. The results obtained disprove a conjecture of J. H. Halton and suggest a conjecture on the improvement of a theorem of Roth.

Key Words: Uniform distribution, equidistribution, distribution functions, diophantine approximation, quadrature, Monte Carlo methods, multiple quadrature, integration, numerical analysis, distribution of points.

1. If $x_1, x_2, \ldots, x_N$ are points in the unit S-dimensional cube G_S, we may approximate to an integral over G_S by the average of the values of the integrand at these points. Writing

$$\int_0^1 \cdots \int_0^1 f(x^{(1)}, x^{(2)}, \ldots, x^{(S)})dx^{(1)} \cdots dx^{(S)} = \frac{1}{N}\sum_{i=1}^{N} f(x_i^{(1)}, \ldots, x_i^{(S)}) + R, \tag{1}$$

(where $x_i^{(1)}, x_i^{(2)} \ldots, x_i^{(S)}$ are the S coordinates of the point x_i), we call R the "error" of the quadrature formula (1). R depends on the integrand f and on the set of points $x_1, \ldots, x_N$; for R to be relatively small for some wide class of functions the set of points should be, in some sense, well distributed in the cube G_S. An appropriate sense of "well distributed" is that, for a region A in G_S, the number of points of the set which lie in A should be approximately N times the volume of A. Restricting attention to regions which are intervals with one vertex at the origin—i.e., which are of the form

$$\{x = (x^{(1)}, \ldots, x^{(S)}) | 0 \leq x^{(i)} < x_0^{(i)}, i = 1, 2, \ldots, S\}$$

for some given $x_0 = (x_0^{(1)}, \ldots, x_0^{(S)}) \epsilon G_S$—we shall let $S_N(x_0^{(1)}, \ldots, x_0^{(S)})$ denote the number of the points $x_1, \ldots x_N$ which lie in such an interval, and consider the quantity $|S_N(x_0^{(1)}, \ldots, x_0^{(S)}) - Nx_0^{(1)}x_0^{(2)}, \ldots x_0^{(S)}|$.

Let

$$D_N^* = D_N^*(x_1, \ldots, x_N) = \sup_{x_0 \epsilon G_S} |S_N(x_0^{(1)}, \ldots, x_0^{(S)}) - Nx_0^{(1)}, \ldots, x_0^{(S)}|. \tag{2}$$

D_N^* is very nearly the "discrepancy" (see, e.g., [1])[1] of the set of N points. E. Hlawka [2] has shown that if the integrand f in (1) is a function of bounded variation and $V(f)$ is its total variation, we have the bound

$$|R| \leq V(f)\frac{D_N^*}{N}. \tag{3}$$

[1] Figures in brackets indicate the literature references at the end of this paper.

Since it is very likely true that all continuous and bounded functions that one ever attempts to integrate numerically are of bounded variation, it is a matter of considerable interest to find sets of points for which D_N^* is as small as possible.

It is easy to see that $D_N^* \geq \frac{1}{2}$. For if $|S_N(x_1^{(1)}, 1, \ldots, 1) - Nx_1^{(1)}| = a < \frac{1}{2}$, then for any $\epsilon > 0$ $|S_N(x_1^{(1)}+\epsilon, 1, \ldots, 1) - N(x_1^{(1)}+\epsilon)| > 1 - a - N\epsilon$ and so is $> \frac{1}{2}$ if ϵ is sufficiently small. In one dimension, the sequence of points $x_i = \dfrac{2i-1}{2N}$, $i = 1, 2, \ldots, N$, has $D_N^* = \frac{1}{2}$ for every N. In two or more dimensions the situation is entirely different; K. F. Roth [3] has shown that for $S > 1$ dimensions there is a positive number $C(S)$ such that

$$D_N^* > C(S)(\log N)^{\frac{S-1}{2}} \tag{4}$$

for any set of N points. It is not known that this result is best possible; there is some reason to guess that the exponent $\dfrac{S-1}{2}$ may be replaceable by $S-1$. In his proof Roth introduced another measure of unevenness of distribution, which we shall denote "E_N". It is defined by

$$E_N = E_N(x_1, \ldots, x_N) = \left(\int_0^1 \cdots \int_0^1 |S_n(x_1^{(1)} \ldots, x^{(S)}) - Nx^{(1)}, \ldots, x^{(S)}|^2 dx^{(1)} \ldots dx^{(S)} \right)^{1/2}. \tag{5}$$

This L^2 norm is sometimes easier to handle than the maximum norm D_N^*, and Roth in fact proved (4) with E_N in place of D_N^*.

In 1935 van der Corput [4] raised the question of whether there exists an infinite sequence $x_1, x_2, \ldots$ of points in the inverval [0, 1] such that $D_N^*(x_1, x_2, \ldots, x_N)$ is bounded in N. This was answered in the negative by Mrs. van Aardenne-Ehrenfest [5] in 1945. Roth, in [3], showed that this problem is equivalent to the problem of estimating a lower bound for D_N^* for fixed N in two dimensions. More generally, Roth showed the existence of a constant C such that: For any N and S, if there is a set of points $x_1, \ldots, x_N$ in G_S such that $D_N^*(x_1, \ldots, x_N) = A$, there is a sequence $x_1', \ldots, x_N'$ in G_{S-1} such that $\max\limits_{n \leq N} D_n^*(x_1', \ldots, x_n') < CA$; and conversely. It follows that for any infinite sequence $x_1, x_2, \ldots$ in [0, 1], $D_N^*(x_1, \ldots, x_N) \geq C'(\log N)^{1/2}$ for infinitely many values of N (where C' is some positive constant). Van der Corput found a sequence for which he showed that $D_N^* \leq \log_2 N + 1$ (here and below "$\log_2$" denotes the logarithm to the base two); it is constructed as follows: for each integer $n \geq 0$, write n as $2^{h_1} + 2^{h_2} + \ldots + 2^{h_k}$ with $h_1 < h_2 < \ldots < h_k$; then $x_n = \frac{1}{2}(2^{-h_1} + 2^{-h_2} + \ldots + 2^{-h_k})$. (We may picture this process as writing n as a numeral to the base 2 and reflecting this numeral in the "decimal point." Thus, in binary notation, $x_0 = 0$, $x_1 = 0.1$, $x_2 = 0.01$, $x_3 = 0.11$, $x_4 = 0.001$, etc.) Roth pointed out that then for each N, the sequence $\left(x_1, \dfrac{1}{N}\right)$, $\left(x_2, \dfrac{2}{N}\right), \ldots, (x_N, 1)$ in G_2 has the property that $D_N^* \leq \log_2 N + 2$. We shall refer to the van der Corput sequence as "$\mathscr{S}$" and to the Roth sequence, for any N, as "$\mathscr{S}'$".

J. M. Hammersley [6] and J. H. Halton [7], interested in the application of evenly distributed sequences to high-dimensional numerical integration, suggested higher-dimensional analogs of these sequences. Defining $\varphi_k(n)$, for any integers $n \geq 0$ and $k > 1$, as the number produced by reflecting the representation of n to the base k in the "decimal point" (more formally, if $n = a_1 k^{h_1} + a_2 k^{h_2} + \ldots a_l k^{h_l}$ where $0 \leq a_i < k$ for $i = 1, \ldots, l$, then $\varphi_k(n) = \dfrac{1}{k}(a_1 k^{-h_1} + \ldots + a_l k^{-h_l})$), Halton suggested the s-dimensional sequence defined by

$$x_n = (\varphi_2(n), \varphi_3(n), \varphi_5(n), \ldots, \varphi_{P_S}(n)), \quad n = 0, 1, 2, \ldots \tag{6}$$

(where P_s is the Sth prime) and Hammersley suggested

$$x_n=\left(\frac{n}{N},\ \varphi_2(n),\ \varphi_3(n),\ \ldots,\ \varphi_{P_{S-1}}(n)\right),\quad n=1,2,\ldots,N. \tag{7}$$

Halton proved that for the sequence (6), D_N^* and E_N are $\leq C(\log N)^K$ and for (7) they are $\leq C'(\log N)^{K-1}$, for some constants C and C'. He further conjectured that the exponents K and $K-1$ could be replaced by $K/2$ and $(K-1)/2$ respectively.

2. In this paper, we shall analyze the distribution of the sequences $\mathscr{S}$ and $\mathscr{S}'$ in detail. Our results are as follows:

THEOREM 1. *For the sequence* $\mathscr{S}$,

$$D_N^*\leq\frac{1}{3}\log_2(N)+0(1) \tag{8}$$

and the constant 1/3 is best possible—that is, with any smaller constant (8) *would not always be true.*

THEOREM 2. *For the sequence* $\mathscr{S}$,

$$E_N\leq\frac{1}{6}\log_2 N+0(1) \tag{9}$$

and the constant 1/6 is best possible.

THEOREM 3. *For the sequence* $\mathscr{S}'$,

$$D_N^*=\frac{1}{3}\log_2 N+0(1). \tag{10}$$

THEOREM 4. *For the sequence* $\mathscr{S}'$,

$$E_N=\frac{1}{8}\log_2 N+0(1). \tag{11}$$

From these theorems it follows that Halton's conjecture is incorrect for the lowest-dimensional cases of his and Hammersley's sequences; it is very likely also to be incorrect in all dimensions.

3. Proofs of the Theorems:

We shall first make some notational conventions.

If a letter is used to represent a nonnegative integer, the same letter may be used to represent the finite string of zeros and ones which is the binary representation of that integer.

If α is a finite string of zeros and ones, we shall enumerate its digits from right to left, calling the rightmost one the "zeroth digit," and write "$\alpha=\alpha_k\ldots\alpha_1\alpha_0$." The number of digits in α will be denoted "$||\alpha||$"; thus $||\alpha_k\alpha_{k-1}\ldots\alpha_0||=k+1$. For $0\leq i\leq k$, "$\alpha^{(i)}$" will denote the string $\alpha_i\alpha_{i-1}\ldots\alpha_1\alpha_0$.

For a string $\alpha=\alpha_k\ldots\alpha_0$, "$.\alpha$" will denote the number $\frac{\alpha_k}{2}+\frac{\alpha_{k-1}}{4}+\ldots+\frac{\alpha_0}{2^{k+1}}$ (if α is null, $.\alpha$ will be taken to be zero). If α and β are strings, "$\alpha\beta$" will denote the string consisting of α and β in the order indicated; so, for example, "0.010α" will denote $\frac{1}{4}+\frac{1}{8}(.\alpha)$, and if $\alpha=1101$, this will be the binary number 0.0101101, or 45/128.

If A is any real number, "$[A]$" will denote the greatest integer not greater than A, and "$\{A\}$" will denote $A-[A]$. The distance from A to the nearest integer, which equals the lesser of $\{A\}$ and $1-\{A\}$, will be denoted "$<A>$."

Let us now fix an integer $N>1$, and set $M=[\log_2 N]$. For any $x\epsilon[0,1]$, let $.a_0a_1a_2\ldots$ be the nonterminating binary representation of x. Let $A=A(x)$ be the string $a_Ma_{M-1}\ldots a_1a_0$. We

will first consider the sequence $\mathscr{S} = x_0, x_1, \ldots,$ with $x_n = \varphi_2(n)$. To estimate $S_n(x)$ we proceed as follows:

For x_n to be less than x, exactly one of the following $M+2$ conditions must hold:

$$(0'.) \quad a_0 > n_0$$

$$(1'.) \quad a_0 = n_0;\ a_1 > n_1$$

$$\vdots$$

$$(M'.) \quad a_0 = n_0,\ a_1 = n_1,\ \ldots,\ a_{M-1} = n_{M-1};\ a_M > n_M$$

$$(M+1'.) \quad a_0 = n_0,\ \ldots,\ a_{M-1} = n_{M-1},\ a_M = n_M.$$

These are equivalent, respectively, to the following conditions:

$$(0.) \quad n \equiv 0 (\mathrm{mod}\ 2),\ a_0 = 1$$

$$(1.) \quad n \equiv a_0 (\mathrm{mod}\ 2^2),\ a_1 = 1$$

$$(2.) \quad n \equiv a_0 + 2a_1 (\mathrm{mod}\ 2^3),\ a_2 = 1$$

$$\vdots$$

$$(M.) \quad n \equiv a_0 + 2a_1 + \ldots + 2^{M-1}a_{M-1} (\mathrm{mod}\ 2^{M+1}),\ a_M = 1$$

$$(M+1.) \quad n \equiv a_0 + 2a_1 + \ldots + 2^M a_M (\mathrm{mod}\ 2^{m+1}).$$

The number of integers $0 \leq n < N$ satisfying condition (0.) is

$$a_0 \left(\left[\frac{N}{2} \right] + 1 \right);$$

the number satisfying condition (1.) is

$$a_1 \left(\left[\frac{N - a_0}{2^2} \right] + 1 \right);$$

the number satisfying condition (2.) is

$$a_2 \left(\left[\frac{N - a_0 - 2a_1}{2^3} \right] + 1 \right);$$

etc. At most one n satisfies condition $M+1$. Thus

$$\sum_{i=0}^{M} a_i \left(\left[\frac{N - (a_0 + 2a_1 + \ldots + 2^{i-1}a_{i-1})}{2^{i+1}} \right] + 1 \right)$$

differs from $S_N(x)$ by at most 1.

Now

$$Nx = N\left(\frac{a_0}{2} + \frac{a_1}{2^2} + \ldots\right) = \sum_{i=0}^{M} a_i \frac{N}{2^{i+1}} + \sum_{i=M+1}^{\infty} a_i \frac{N}{2^{i+1}}.$$

By the definition of M the second sum is between zero and 1. If we now set

$$d = d(x, N) = \sum_{i=0}^{M} a_i \left(\left[\frac{N - (a_0 + \ldots + 2^{i-1}a_{i-1})}{2^{i+1}} \right] + 1 - \frac{N}{2^{i+1}} \right), \tag{12}$$

then d differs from $S_N(x) - Nx$ by at most 2; and so in proving our Theorems, for which a difference which is 0(1) has no effect, we may deal with d instead of $S_N(x) - Nx$ throughout.

Now

$$\frac{a_0 + 2a_1 + \ldots + 2^{i-1}a_{i-1}}{2^{i+1}} = .0a_{i-1}a_{i-2} \ldots a_0$$

(in binary notation), and may be written "$.0A^{(i-1)}$"; it is equal to $\frac{1}{2}\varphi_2([2^i x])$. $\left\{ \frac{N}{2^{i+1}} \right\}$ may also be written "$.N^{(i)}$." Since

$$\left[\frac{N - (a_0 + \ldots + 2^{i-1}a_{i-1})}{2^{i+1}} \right] + 1 - \frac{N}{2^{i+1}} = \left[\left[\frac{N}{2^{i+1}} \right] + (.N^{(i)} - .0A^{(i-1)}) \right] - \left[\frac{N}{2^{i+1}} \right] + 1 - .N^{(i)},$$

we may write

$$d = \sum_{i=0}^{M} a_i b_i, \text{ where } b_i = \begin{cases} 1 - .N^{(i)} \text{ if } .N^{(i)} \geq .0A^{(i-1)} \\ -.N^{(i)} \text{ if } .N^{(i)} < .0A^{(i-1)}. \end{cases} \tag{13}$$

We will first obtain a lower bound for d: $b_i < 0$ only if $N_i = 0$; therefore

$$d \geq \sum_{\substack{N_i = 0 \\ 0 \leq i \leq M}} a_i b_i \geq - \sum_{\substack{N_i = 0 \\ 0 \leq i \leq M}} b_i \geq - \sum_{\substack{N_i = 0 \\ 0 \leq i \leq M}} .N^{(i)}. \tag{14}$$

To estimate this last sum, we first note that if the string N (read from right to left) starts with a block of consecutive zeros, the $.N^{(i)}$ corresponding to those digits are zero; and so that block of zeros may be removed from N. Similarly a block of ones occurring at the leftmost end of N may be removed. What remains of N can then be broken into disjoint substrings of the forms 01, 001, 0001, . . . and 1, 11, 111, ... A substring 01 contributes one term to the sum $-.N^{(i)}$ for that i which is the index of the zero in the substring. Since that $.N^{(i)}$ is less than 1/2, the contribution of such a substring to the sum is less than 1/4 the length of the substring. Similarly each block of the form 001, 0001, . . . contributes to the sum a set of terms whose total is less than 1/4 the length of the block. Substrings of the form 1, 11, 111, . . . contribute nothing to the sum. It follows that

$$d > -\frac{M+1}{4}. \tag{15}$$

To obtain a sharp upper bound on d we shall require some lemmas:

LEMMA 1. *For a fixed integer* $M \geq 1$ *and real number* $x \in [0,1]$, *and* $A = A(x)$ *as defined above, the maximum of* $d(x, N)$ *over all* N *between* 0 *and* $2^{M+1} - 1$, *is attained at* $N = 2A - 2^{M+1}a_M$. (*i.e.*, $N_0 = 0$, $N_i = a_{i-1}$ *for* $i = 1, 2, \ldots, M$.)

PROOF: $d(x, N)=\sum_{i=0}^{M} a_i(x)b_i(x, N)$. Changing any digit N_i of N changes b_j only for $j \geq i$. If a change in some N_i does not change the sign of some b_j, $j \geq i$, then it changes that b_j by just $\frac{1}{2^{j-i+1}}$. For any i between 0 and M, let j_0 be the 1'st $j \geq i$ such that $a_j = 1$; it then follows that if changing N_i does not change the sign of b_j for any $j \geq 1$, the change in $a_{j_0}b_{j_0}$ dominates the sum of all the changes in d resulting from the change in N_i. On the other hand, no b_i with $j \geq i$ changes sign unless b_{j_0} does; so if the change in N_i does change the sign of some b_j, the change in $a_{j_0}b_{j_0}$ is still dominating. It follows that the N that maximizes d must also maximize $\sum_{i=0}^{K} a_ib_i$ for every K between zero and M.

Now let $a_{r_1}, a_{r_2} \ldots (r_i < r_2 < \ldots)$, be the 1's in A. To maximize $\sum_{i=0}^{r_1} a_ib_i$ we must clearly set $N_0 = N_1 = \ldots = N_{r_1} = 0$. Proceeding by induction, we assume that $N_i = a_{i-1}$ for $i = 1, 2, \ldots, r_k$, and try to define $N_{r_k+1}, \ldots, N_{r_{k+1}}$ so as to maximize $\sum_{i=0}^{r_{k+1}} a_ib_i$. If $r_{k+1} = r_k + 1$, we must set $N_{r_k+1} = 1$, for otherwise b_{r_k+1} would be negative. If $r_{k+1} > r_k + 1$, it is clear that $b_{r_{k+1}}$ is maximized by setting $N_{r_k+1} = 1$, $N_{r_k+2} = N_{r_k+3} = \ldots = N_{r_{k+1}} = 0$. In either case $N_i = a_{i-1}$ for $i = r_k + 1, \ldots, r_{k+1}$, proving the lemma.

Let us now, for any finite string α of zeros and ones, let $\delta(\alpha)$ be the maximum of $d(x, N)$ for $0 \leq N < 2^{\|\alpha\|+1}$ and $A(x) = \alpha$. It remains to determine the maximum of $\delta(\alpha)$ over all strings α of a given length.

For any integer $L \geq 1$, let σ_L and σ'_L be the strings 10101 . . . 01 and 0101 . . . 01011, respectively, each of length $2L + 1$ ($\sigma_1 = 101$, $\sigma'_1 = 011$).

LEMMA 2. *If $0 \leq t \leq 1$, the maximum of $\delta(\alpha) - t(.\alpha)$ over all strings α of length $2L + 1$ occurs at $\alpha = \sigma_L$; if $1 \leq t \leq 2$ the maximum occurs at $\alpha = \sigma'_L$.*

PROOF: We first note that $\delta(\sigma'_L) = \frac{2}{3}L + \frac{7}{9} + \frac{2}{9 \cdot 4^L}$; and that $.\sigma_L = \frac{2}{3} - \frac{1}{6 \cdot 4^L}$ and $.\sigma'_L = \frac{1}{3} + \frac{1}{6 \cdot 4^L}$. The proof proceeds by induction on L. For $L = 1$ the lemma is shown true by direct calculation. Assuming it true for L, if α is a string of length $2(L + 1) + 1$, then $\alpha = 00\beta$ or 01β or 10β or 11β, where $\|\beta\| = 2L + 1$. In these 4 cases respectively we have:

$$\delta(\alpha) - t(.\alpha) = \delta(\beta) - \frac{t}{4}(.\beta)$$

$$\delta(\beta) - \left(1 + \frac{t}{4}\right)(.\beta) + 1 - t/4$$

$$\delta(\beta) - \left(\frac{1}{2} + \frac{t}{4}\right)(.\beta) + 1 - t/2$$

$$\delta(\beta) - \left(\frac{3}{2} + \frac{t}{4}\right)(.\beta) + \frac{3}{2} - \frac{3t}{4};$$

we shall call these quantities δ_1, δ_2, δ_3, and δ_4. By the induction hypothesis, for $0 \leq t \leq 2$, δ_1 and δ_3 are maximized by taking $\beta = \sigma_L$, and δ_2 and δ_4 are maximized by $\beta = \sigma'_L$. Direct calculation then shows that δ_3 is the largest of the four when $0 \leq t \leq 1$, and δ_2 is largest when $1 \leq t \leq 2$, which proves the lemma.

Thus in particular the maximum of $\delta(\alpha)$ over all strings α of length $2L + 1$ is $\delta(\sigma_L)$, which is equal to $\frac{1}{3}\|\alpha\| + 0(1)$.

Furthermore, if α is a string of even length then $\alpha = 0\beta$ or 1β, where $\|\beta\| = 2L + 1$ for some integer L. In the first case $\delta(\alpha) = \delta(\beta)$, and in the second $\delta(\alpha) = 1 - .\beta + \delta(\beta)$. Since $.\beta < 1$, $\alpha = 1\beta$

yields the larger δ, and then, by Lemma 2., $\delta(\alpha)$ is maximal when $\beta=\sigma_L$ or σ_L'; and once again the maximum of $\delta(\alpha)$ is $\frac{1}{3}\|\alpha\|+0(1)$.

Lemmas 1 and 2 together imply that for any positive integer M the maximum of $d(x, N)$ for $0\leq x\leq 1$ and $0\leq N<2^{M+1}$ is $\frac{M+1}{3}+0(1)$, and Theorem 1. follows.

To prove Theorem 2., we shall first show:

LEMMA 3. $$\left(\int_0^1 (S_N(x)-Nx)^2\,dx\right)^{1/2}=\frac{1}{2}\sum_{i=1}^{\infty}\left\langle\frac{N}{2^i}\right\rangle+0(1).$$

PROOF: First of all, it is sufficient to prove the equation with $d(x, N)$ in place of $S_N(x)-Nx$. For fixed N, and $i=0,1,\ldots, M$ let $f_i(x)=a_i(x)b_i(x, N)$. Then $d(x, N)=f_0(x)+f_1(x)+\ldots+f_M(x)$, and

$$\int_0^1 d^2(x, N)dx=\left(\sum_{i=0}^{M}\int_0^1 f_i\right)^2+\sum_{i=0}^{M}\left(\int_0^1 f_i^2-\left(\int_0^1 f_i\right)^2\right)+2\sum_{0\leq i<j\leq M}\left(\int_0^1 f_if_j-\int_0^1 f_i\int_0^1 f_j\right). \quad (16)$$

To evaluate the first term on the right of (16), we first define C_i, for each i, by

$$C_i(x)=\begin{cases}1-.N^{(i)} \text{ if } .N^{(i)}\geq .0A^{(i+1)}+\frac{1}{2^{i+1}}\\ -.N^{(i)} \text{ otherwise}\end{cases} \quad (17)$$

and note that $C_i=b_i$ unless $.0A^{(i-1)}\leq .N^{(i)}<.0A^{(i-1)}+\frac{1}{2^{i+1}}$, when $C_i=b_i-1$. Now $.0A^{(i-1)}=\frac{1}{2}\varphi_2([2^ix])$ and so is constant on each interval $\left(\frac{r}{2^i}, \frac{r+1}{2^i}\right)$, $r=0, 1, \ldots, 2^i-1$; and its values on different intervals differ by at least 2^{-i}. Thus C_i and b_i are equal everywhere except perhaps on one interval of length 2^{-i}, so that if we set $F_i(x)=a_i(x)C_i(x)$, we have

$$\int_0^1 |F_i(x)-f_i(x)|dx\leq\frac{1}{2^i}, \text{ and } \left|\sum_{i=0}^{M}\int_0^1 F_i-\sum_{i=0}^{M}\int_0^1 f_i\right|\leq 2. \quad (18)$$

Since a_i is zero on one half of each interval $\left(\frac{r}{2^i}, \frac{r+1}{2^i}\right)$ and one on the other half, while C_i is constant on the interval, $\int_0^1 F_i(x)dx=\frac{1}{2}\int_0^1 C_i(x)dx$. The values $.0A^{(i-1)}+\frac{1}{2^{i+1}}$ takes on these 2^i intervals are just the numbers $\frac{1}{2^{i+1}}, \frac{2}{2^{i+1}}, \ldots, \frac{2^i}{2^{i+1}}$. So if $.N^{(i)}\geq\frac{1}{2}$, $C_i=1-.N^{(i)}$ throughout (0,1) and $\int_0^1 F_i=\frac{1}{2}(1-.N^{(i)})=\frac{1}{2}\left\langle\frac{N}{2^{i+1}}\right\rangle$. If $.N^{(i)}<\frac{1}{2}$, we may write $.N^{(i)}=K/2^{i+1}$, where K is an integer between 0 and 2^i-1. It's then easy to see that $.N^{(i)}<.0A^{(i-1)}+\frac{1}{2^{i+1}}$ on just 2^i-K of the above intervals. Then $C_i(x)=.N^{(i)}$ on a set of measure $1-K/2^i$ and $1-.N^{(i)}$ on a set of measure $K/2^i$; so that $\int_0^1 F_i=\frac{.N^{(i)}}{2}=\frac{1}{2}\left\langle\frac{N}{2^{i+1}}\right\rangle$ once again. Therefore, by (18),

$$\sum_{i=0}^{M}\int_0^1 f_i=\frac{1}{2}\sum_{i=0}^{M}\left\langle\frac{N}{2^{i+1}}\right\rangle+0(1)=\frac{1}{2}\sum_{i=1}^{\infty}\left\langle\frac{N}{2^i}\right\rangle+0(1). \quad (19)$$

Lemma 3. will now follow if we show that the second and third terms on the right in (16) are

each $O(\log N)$. For the second term this is obvious, since $|f_i(x)| \leq 1$. To bound the 3d term we proceed as follows:

For $0 \leq i \leq M$, set $b_i(x) = -.N^{(i)} + e_i(x)$, and $y_i(x) = .0A^{(i-1)}$.

Then

$$e_i = \begin{cases} 1 \text{ if } .N^{(i)} \geq y_i \\ 0 \text{ if } .N^{i} < y_i \end{cases}, \tag{20}$$

and

$$\int_0^1 f_i f_j - \int_0^1 f_i \int_0^1 f_j = \frac{1}{4}\left(\int_0^1 e_i e_j - \int_0^1 e_i \int_0^1 e_i\right). \tag{21}$$

Now for any i and j, $i < j$, set $z_{i,j}(x) = y_j(x) - 2^{i-j} y_i(x)$. Recalling that $y_i = \frac{1}{2}\varphi_2([2^i x])$ and noting that $\varphi_2([2^i x]) = \{2^{j-i}\varphi_2([2^j x])\}$, we see that $z_{j,i}$ takes on, in each interval $\left(\frac{r}{2^i}, \frac{r+1}{2^i}\right)$, the 2^{j-i} values $\frac{l}{2^{j-i+1}}$, $l = 0,1, \ldots, 2^{j-i} - 1$; and each value is taken on an interval of length 2^{-j}. Therefore $z_{j,i}$, and y_i are independent functions of x, and if we define $e_j^*(x) = e_{j,i}^*(x)$ by

$$e_j^* = \begin{cases} 1 \text{ if } .N^{(i)} \geq z_j \\ 0 \text{ if } .N^{(i)} < z_j \end{cases}, \tag{22}$$

we can conclude that

$$\int_0^1 e_i e_j^* - \int_0^1 e_i \int_0^1 e_j^* = 0. \tag{23}$$

By reasoning as we did above about b_i and C_i we can see that $e_i(x)$ and $e_j^*(x)$ are equal except on a set of measure at most 2^{i-j+1}, and there $|e_j^*(x) - e_j(x)| = 1$. Therefore, by (23)

$$\left|\int_0^1 e_i e_j - \int_0^1 e_i \int_0^1 e_j\right| = \left|\int_0^1 e_i(e_j - e_j^*) - \int_0^1 e_i \int_0^1 (e_j - e_j^*)\right| \leq 2\int_0^1 \left|e_j - e_j^*\right| \leq \frac{4}{2^{j-i}}.$$

From (21), therefore,

$$\sum_{0 \leq i < j \leq M} \left(\int_0^1 f_i f_j - \int_0^1 f_i \int_0^1 f_j\right) \leq \sum_{0 \leq i < j \leq M} \frac{1}{2^{i-j}} < M,$$

which completes the proof of the lemma.

To prove Theorem 2 we must now show that

$$\sum_{i=0}^{M} \left\langle \frac{N}{2^{i+1}} \right\rangle \leq \frac{1}{3}\log_2 N + O(1), \tag{24}$$

and that the constant 1/3 in (24) is best possible. We have seen that $\sum_{i=0}^{M} \left\langle \frac{N}{2^{i+1}} \right\rangle = \sum_{i=0}^{M} \min(.N^{(i)}, 1 - .N^{(i)})$; and we shall show that the last sum is maximized (over all $0 \leq N < 2^{M+1}$) when N is of the form . . . 010101:

For $M = 0$, this is obvious. If $M = K$, then $N = 0N'$ or $1N'$, where N' is a string with $M = K - 1$. In the first case the sum is $\frac{1}{2}(.N') + \sum_{i=0}^{K-1} \min(.N^{(i)}, 1 - .N^{(i)})$, and in the second it is $\frac{1}{2}(1 - .N') + \sum_{i=0}^{K-1}$

min $(.N^{(i)}, 1-.N^{(i)})$. The first is larger if the leftmost digit of N' is 1, while the second is larger if the leftmost digit of N' is zero; which completes the induction. For N of the form specified, $\sum_{i=0}^{M}\left\langle\frac{N}{2^{i+1}}\right\rangle$ is equal to $1/3\log_2 N+0(1)$, so (24) is established, together with the fact that the constant 1/3 cannot be improved upon.

To derive Theorems 3 and 4 from Theorems 1 and 2 we will use a device of K. F. Roth [3]. For any N, and $0\leq x\leq 1$ and $0\leq y\leq 1$, let $n=n(y)=[Ny]$. Then $S_N(x, y)$ for the sequence $\mathscr{S}'$ is equal to $S_n(x)$ for the sequence $\mathscr{S}$. Furthermore $|N xy-nx|\leq 1$, so that

$$\sup_{0\leq x,\, y\leq 1}|S_N(x, y)-Nxy| \text{ differs from } \sup_{\substack{0\leq x\leq 1\\ 0<n<N}}|S_n(x)-nx| \text{ by no more}$$

than 1. From Theorem 1,

$$|S_n(x)-nx|\leq\frac{1}{3}\log_2 n+0(1)\leq\frac{1}{3}\log_2 N+0(1);$$

and from the proof of Theorem 1, if n is the largest integer between 0 and N whose binary representation is of the form 10101 . . . 01,

$$\sup|S_n(x)-nx|=\frac{1}{3}\ \|n\|\ +0(1)=\frac{1}{3}\ \|N\|\ +0(1).$$

Theorem 3 follows.

To prove Theorem 4. we use the device of Roth to replace

$$\left(\int_0^1\int_0^1(S_N(x, y)-Nxy)^2dydy\right)^{1/2}\ \text{by}\ \left(\int_0^1\int_0^1(S_{n(y)}(x)-xn(y))^2dx\,dy\right)^{1/2};$$

the latter, in turn, differs by only 0(1) from

$$\left(\int_0^1\left(\frac{1}{2}\sum_{i=0}^{M}\left\langle\frac{n(y)}{2^{i+1}}\right\rangle\right)^2dy\right)^{1/2}. \tag{25}$$

Setting $g_i(y)=\left\langle\frac{n(y)}{2^{i+1}}\right\rangle$, we can write

$$\int_0^1\left(\sum_{i=0}^{M}\left\langle\frac{n}{2^{i+1}}\right\rangle\right)^2dy=\left(\sum_{i=0}^{M}\int_0^1 g_i\right)^2+\sum_{i=0}^{M}\left(\int_0^1 g_i^2-\left(\int_0^1 g_i\right)^2\right)+2\sum_{0\leq i<j\leq M}\left(\int_0^1 g_ig_j-\int_0^1 g_i\int_0^1 g_j\right). \tag{26}$$

As in the analysis of (16), we wish to show that the second and third terms on the right of (26) are each $0(M)$. For the second this is obvious; for the third we proceed so: For each i and $j>i$, set $g_{j.i}(y)=\left\langle\left\{\frac{n}{2^j}\right\}-2^{i-j}\left\{\frac{n}{2^i}\right\}\right\rangle$; $g_{j.i}$ is then a function of only the $M-j$th through $M-i+1$th digits of the binary representation of y, and so is independent of g_i, which is a function of the $M-i$th through Mth digits. Furthermore $\int_0^1|g_{j.i}(x)-g_j(x)|dx\leq\frac{2}{2^{j-i}}$; that the third term is $0(M)$ follows as in the proof of Lemma 3.

To evaluate the first term on the right of (26), we note that

$$\int_0^1 g_i(y)dy=\int_0^1\frac{[Ny]}{2^{i+1}}dy=\frac{1}{N}\sum_{r=0}^{N-1}\left\langle\frac{r}{2^{i+1}}\right\rangle. \tag{27}$$

211-570 O-66—2

Since $\langle x \rangle = \langle \{x\} \rangle$, the sum in (27) can be written as

$$\left[\frac{N}{2^{i+1}}\right] \sum_{r=0}^{2^{i+1}-1} \left\langle \frac{r}{2^{i+1}} \right\rangle + E_i = \frac{2^{i+1}}{4}\left[\frac{N}{2^{i+1}}\right] + E_i, \tag{28}$$

where

$$0 \leq E_i = \sum_{r=2^{i+1}\left[\frac{N}{2^{i+1}}\right]}^{N-1} \left\langle \frac{r}{2^{i+1}} \right\rangle < \frac{2^{i+1}}{4}. \tag{29}$$

Therefore

$$N\int_0^1 g_i = \frac{2^{i+1}}{4}\left(\frac{N}{2^{i+1}} - \left\{\frac{N}{2^{i+1}}\right\} + \frac{4}{2^{i+1}}E_i\right) \tag{30}$$

$$= \frac{N}{4} + \frac{2^{i+1}}{4}\theta_i,$$

where $|\theta_i| \leq 1$.

So

$$\sum_{i=0}^{M}\int_0^1 g_i = \frac{M+1}{4} + \frac{\theta}{N}\sum_{i=0}^{M} 2^{i-1} \tag{31}$$

where $|\theta| < 1$. Since $\sum_{i=0}^{M} 2^{i-1} < 2^M \leq N$, we can conclude that

$$\sum_{i=0}^{M}\int_0^1 g_i = \frac{M}{4} + 0(1) \tag{32}$$

and Theorem 4. follows.

4. An attempt to analyze the higher-dimensional sequences of Hammersley and Halton along the above lines was unsuccessful, due to the greater complication of those sequences. Analogs, for those sequences, of Theorems 1 and 3 would be very useful in application of the sequences to multiple numerical quadrature.

Intuitively, van der Corput's sequence $\mathscr{S}$ seems to be about as evenly distributed as possible. This feeling, together with Theorem 1, leads us to the conjecture in section 1 that K. F. Roth's lower bound on D_N^* can be improved.

References

[1] J. W. S. Cassels, An Introduction to Diophantine Approximation (Cambridge University Press, 1957).

[2] E. Hlawka, Funktionen von beschrankter Variation in der Theorie der Gleichverteilung. Annali di Matematica (IV) 54, 1961.

[3] K. F. Roth, On irregularities of distribution, Mathematika **1** (1954).

[4] J. G. van der Corput, Verteilungsfunktionen, Proc. Kon. Ned. Akad. v. Wetensch., Section of Sciences **38** (1935).

[5] T. van Aardenne-Ehrenfest, Proof of the impossibility of a just distribution of an infinite sequence of points over an interval, Proc. Kon. Ned. Akad. v. Wetensch. **48** (1945).

[6] J. M. Hammersley, Monte Carlo methods for solving multivariable problems, Annals of the New York Academy of Sciences, **86** (1960).

[7] J. H. Halton, On the efficiency of certain quasi-random sequences of points in evaluating multi-dimensional integrals. Numerische Math. **2**, 1960.

(Paper 70B2–172)

JOURNAL OF RESEARCH of the National Bureau of Standards – B. Mathematics and Mathematical Physics
Vol. 70B, No. 2, April–June 1966

On Abstract Numerical Integrations

John J. Sopka*

National Bureau of Standards, Boulder, Colo.

(March 10, 1966)

Let X be a space of functions, say $X \subset C(K)$, K locally compact Hausdorff, let $l \epsilon X^*$ be an integral on X and let $M^* \subset X^*$ be a given subspace of "simple" functionals, then it is desired to obtain an $\bar{l} \epsilon M^*$ for given n, $\bar{l} \epsilon M_n^* \subset M^*$; M_n^* being a suitable n dimensional subspace determined so that $l - \bar{l}$ annihilates a given finite dimensional subspace $X_1 \subset X$. In this general context, the abstract analysis of numerical integration is developed and certain specific applications are made.

Key Words: Numerical integrations, abstract Gaussian quadrature methods.

1. Introduction

In the development of numerical integration formulas, one is given a function space X, say $X \subset C(K)$, where K is some locally compact Hausdorff space, and an integral $l \epsilon X^*$. It is then desired to find an $\bar{l} \epsilon M^* \subset X^*$, where M^* is a subspace generated by a family of "simple" integrals $\{x_\alpha^*\}$ such that $\bar{l}$ can be said to approximate l in some given sense.

In ordinary quadrature, the family $\{x_\alpha^*\}$ are given by $x_\alpha^* f = f(x_\alpha) \forall f \epsilon C(K)$ where $x_\alpha \epsilon K$. An element $\bar{l} \epsilon M^*$ is said to approximate the given integral l if $l - \bar{l} \epsilon X_\omega^\perp$ where $X_\omega^\perp$ is the subspace in X^* of all annihillators of a given subspace $X_\omega \subset X$.

The following paper summarizes the essential mathematical structure of numerical integration methods with the purpose of extending systematically the class of such methods.

2. General Analysis

Let $X \subset C(K)$ and let $X_0 \subset X$ be a subspace ∋ dim $X_0 = n$ and X_0 is generated by a given set of n "basis" functions $\{f_k\}$. In X^* take M^* a subspace generated by a given family $\{x_\alpha^*\}$ of linearly independent functionals with the properties: M^* is total over X_0 and $\{x_\alpha^*\} \cap X_0^\perp$ is void where $X_0^\perp = \{l;\ l \epsilon X^*,\ lf = 0,\ f \epsilon X_0\}$. If $M_n^* \subset M^*$ designates a subspace generated by n of the x_α^*, say $\{x_{\alpha i}\}\ i = 1 \ldots n$ so that dim $M_n^* = n$, then one has $X^* = X_0^\perp + M_n^*$ since the deficiency of $X_0^\perp$ = dim $X_0 = n$. Also M_n^* is total over X_0 as is readily seen.

If $l \epsilon X^*$ is a given integral, then ∄ $\bar{l} \epsilon M_n^*$ ∋ $l = \bar{l} + l_0^\perp$ where $l_0^\perp \epsilon X_0^\perp$ and ∄ such an $\bar{l}$ for each subspace M_n^* as defined above. For any such given subspace M_n^* ∄ $l_i \epsilon M_n^*$ $i = 1 \ldots n$ ∋ $l_i f_k = \delta_{ik}$ $i, k = 1 \ldots n$ $\delta_{ik} = 1$ $i = k$, $\delta_{ik} = 0$ $i \neq k$. This follows from M_n^* being total over X_0.

Thus one can write: $l = \sum_i l(f_i)\, l_i + l_0^\perp$, $l_0^\perp \epsilon X_0^\perp$ and $l_i = \sum_j \gamma_{ij} x_j^*$ where $x_j^* = x_{\alpha_j}^*$.

Then
$$l = \sum_i \sum_j (lf_i)\gamma_{ij} x_j^* + l_0^\perp$$

or
$$\bar{l} = l - l_0^\perp = \sum_j \left(\sum_i lf_i \gamma_{ij} \right) x_j^*. \tag{1}$$

The functional $\bar{l}$ therefore depends on the selected set $\{x_{\alpha i}^*\}$, that is on M_n^*, on the lf_i and on the coefficients γ_{ij} $i, j = 1 \ldots n$.

The relations $\sum_j \gamma_{ij} x_j^* f_k = \delta_{ik} i$, $k = 1 \ldots n$ can be put in matrix form: $\Gamma \Gamma_0 = I$ where I is the identity matrix, $\Gamma = (\gamma_{ij})$ $\Gamma_0 = (x_j^* f_k)$. Now Γ_0 is nonsingular for any given M_n^* since M_n^* total over X_0 implies that $\sum_{k=1}^{n} \tau_k x_j^* f_k = 0$ $j = 1 \ldots n$ is possible only when $\tau_k = 0$ $k = 1 \ldots n$. Hence the matrix $\Gamma = \Gamma_0^{-1}$ is determined once Γ_0 is known.

If the $\{f_k\}$ are such that the lf_k are readily evaluated then the problem of determining $\bar{l}$ is that of specifying M_n^* or a corresponding basis $\{x_{\alpha i}^*\}$. Under the conditions imposed thus far with dim X_0 = dim $M_n^* = n$ $\bar{l}$ will not in general be unique without additional conditions on X and/or the M_n^*.

3. Specific Cases

In certain quadrature procedures, such as the Newton-Cotes formulas, M_n^* is specified a priori by choosing the $x_{\alpha i}^*$. The subspace X_0 in these cases is such that the lf_i are easily calculated and thus $\bar{l}$

*Consultant-Mathematics, National Bureau of Standards, Boulder, Colo.

is determined. For instance, the Parabolic Rule has $l=\int_{x_1}^{x_3} dx$, where X_0 is the space over the Reals generated by the $f_k=x^{k-1}$, $k=1,2,3$ and $x_{ai}^*f=f(x_i)$ for given real numbers x_1, $x_2=\frac{1}{2}(x_1+x_3)$, x_3.

In Gaussian quadrature methods, the following additional conditions limit the choice of M_n^*. Consider a subspace $X_1 \subset X$, where $X_1 \supset X_0$ and X_1 has generators $\{f_k'\}$, $k=1 \ . \ . \ . \ p$, $p>n$, $f_k'=f_k$ for $k=1 \ . \ . \ . \ n$. Now if T is a linear transformation on $X \ni f_k'=Tf_{k-1}'=T^{k-1}f_1'$. Then T induces a linear transformation Q on X^* given by $Ql f=lf=lTf$, $\forall l \epsilon X^*$, $f \epsilon X$. Consequently $x_j^*f_k'=(Qx_j^*)f_{k-1}'=(Q^{k-1}x^*)f_1'$ and one can write:

$$\bar{l}f_k=\sum_j\left(\sum_i lf_i\gamma_{ij}\right)Q^{k-1}x_j^*f_1 \text{ for } k=1 \ . \ . \ . \ p. \tag{2}$$

Since the matrix $\Gamma_0=(x_j^*f_k)=(Q^{k-1}x_j^*f_1)$ for $j, k=1 \ . \ . \ . \ n$ is nonsingular, the n-tuple $(Q^nx_j^*f_1)$ $j=1 \ . \ . \ . \ n$ corresponding to

$$\bar{l}f_{n+1}=\sum_j\left(\sum_i lf_i\gamma_{ij}\right)Q^nx_j^*f_1$$

is linearly dependent on the rows of Γ_0, i.e.

$$Q^nx_j^*f_1=\sum_{k=1}^n\beta_kQ^{k-1}x_j^*f_1 \qquad j=1 \ . \ . \ . \ n. \tag{3}$$

This gives the relationship

$$\bar{l}f_{n+1}'=\sum_{k=1}^n\beta_k\bar{l}f_k'. \tag{4}$$

Now, if for $M_{n\perp}^*=\{f;\ f \epsilon X_1,\ x_j^*f=0,\ j=1 \ . \ . \ . \ n\}$ one also assumes: $TM_{n\perp}^* \subset M_{n\perp}^*$ that is, $x_j^*f=0$ implies $x_j^*Tf=0=Qx_j^*f$ for $j=1 \ . \ . \ . \ n$ then this condition, plus the statement:

$$\left(Q^n-\sum_{i=1}^n\beta_kQ^{k-1}\right)x_j^*f_1'=0 \qquad j=1 \ . \ . \ . \ n \tag{5}$$

will imply that

$$\left(Q^{n+q}-\sum_{k=1}^n\beta_kQ^{k+q-1}\right)x_j^*f_1'=0 \qquad j=1 \ . \ . \ . \ n, \forall q \tag{6}$$

Taking $q=0, 1 \ . \ . \ . \ n-1$ one gets the n equations

$$\bar{l}f_{n+1+q}'=\sum_{k=1}^n\beta_k\bar{l}f_{k+q}' \tag{7}$$

In Gaussian quadrature, the stronger condition $l-\bar{l} \epsilon X_1^\perp \subset X_0^\perp$ is imposed. Thus, if $l-\bar{l} \epsilon X_1^\perp$, if the f_{k+q}' are such that the lf_{k+q}' are readily obtained and if the matrix $L=(lf_{k+q}')$, $k=1 \ . \ . \ . \ n$, $q=0 \ . \ . \ . \ n-1$ is nonsingular then the β_k can be obtained uniquely. Given the β_k, solution for the $x_j^*f_1'$ $j=1 \ . \ . \ . \ n$ follows from the relations (5) when they are solvable. Determination of the functionals x_j^* $j=1 \ . \ . \ . \ n$ proceeds from the values of the $x_j^*f_1$ when the x_j^* are sufficiently simple, for example, a one parameter family like those in the examples below.

Now, $L=(lf_{k+q}')$ is nonsingular if and only if $\nexists$ scalars

$$\epsilon_k \neq 0,\ k=1 \ . \ . \ . \ n \ni l\left(\sum_{k=1}^n \epsilon_k f_{k+q}\right)=0$$

$$q=0 \ . \ . \ . \ n-1.$$

Since these last relations can be written as:

$$l\left(\sum_{k=1}^n \epsilon_k T^{k-1+q}f_1\right)=l\left(T^q\left(\sum_{k=1}^n \epsilon_k T^{k-1}\right)f_1\right)=0 \tag{8}$$

one has, in this general context, an orthogonality condition stating that no $n-1$ degree "polynomial" in T is orthogonal in this sense to all $n-1$ degree polynomials in T. The n-equations (7) can also be written as:

$$l\left(T^q\left(T^n-\sum_{k=1}^n\beta_kT^{k-1}\right)f_1\right)=0 \qquad q=0 \ . \ . \ . \ n-1 \tag{9}$$

which states that the n degree polynomial $T^n-\sum_{k=1}^n\beta_kT^{k-1}$ is orthogonal, in this sense, to all $n-1$ degree polynomials in T.

Thus if X_0, X_1, M_n^* satisfy the conditions imposed, it was seen in the general section above that $\exists \bar{l} \epsilon M_n^* \ni l-\bar{l} \epsilon X_0^\perp$. The preceding discussion shows that if $l-\bar{l} \epsilon X_1^\perp$ then (9) follows. Conversely, if $\exists\ \beta_k \ni$ (9) holds one shows directly $l-l \epsilon X_1^\perp$ using (5) and (6). Consequently one has the following statement analogous to the ordinary Gaussian quadrature theorem [1] which is usually stated in terms of classical orthogonal polynomials: If X_0, X_1, M_n^* satisfy all the conditions imposed above then $\exists \bar{l} \epsilon M_n^* \ni l-\bar{l} \epsilon X_1^\perp$ if and only if $\exists$ an n degree "polynomial" $T^n-\sum_{k=1}^n\beta_kT^{k-1}$ orthogonal as in (9) to all polynomials in T of degree $<n$.

4. Applications

In ordinary Gaussian quadrature, the above specializes to the case where $X_0=\{x^{i-1};\ i=1 \ . \ . \ . \ n\}$, $X_1=\{x^{i-1};\ i=1 \ . \ . \ . \ 2n\}$, and the $\{x_a^*\}$ are defined by $x_a^*f=f(x_a)$. Then the other Gaussian conditions are seen to hold when T is $\ni(Tf)(x)=f(x)x$.

An interesting nonclassical application is to $l=\int_0^1 dx$ on the space $X=C_0(K)=\{f;\ f \epsilon C(K),\ K=[0,1], f(0)=f(1)=0\}$. The natural basis functions here are $\sin \pi kx$ or the equivalent functions $f_k(x)=\sin \pi x\ (\cos \pi x)^{k-1}$.

Take X_0, X_1, with this basis and x_α^* defined by $x_\alpha^* f = f(x_\alpha)$, $x_\alpha \epsilon [0, 1]$. Take $T \ni Tf(x) = f(x) \cos \pi x$ then $TM_{n\perp}^* \subset M_{n\perp}^*$ and one gets:

$$\bar{l} = 0.39\,(x_1^* + x_2^*) \qquad \text{for } n = 2$$

$$\bar{l} = 0.205\,(x_1^* + x_3^*) + 0.247\,(x_2^* + x_4^*) \qquad \text{for } n = 4$$

$$\bar{l} = 0.18502\,(x_1^* + x_2^*) + 0.12306\,(x_3^* + x_4^*) + 0.16882\,(x_5^* + x_6^*) \qquad \text{for } n = 6.$$

Another application is to $l = \int_0^\infty k(x)dx$ for some weight function $k(x)$ e.g., $k(x) = e^{-x^2}$. Here $K = [0, \infty]$

$$X = \left\{ f;\ f \epsilon C(K),\ lf \text{ exists},\ \int_0^x f(t)dt \text{ exists and is easily obtained for arbitrary } x \epsilon K \right\}.$$

Take $f_k'(x) = kx^{k-1}$, let $x_j^* f = k(\xi_j) \int_{x_{j-1}}^{x_j} f(x)dx$. For $x_0 = 0$ $x_{j-1} < \xi_j < x_j$ and take T given by $Tf(x) = xf(x) + \int_0^x f(t)dt$ then $TM_{n\perp}^* \subset M_{n\perp}^*$ and one gets:

$$\bar{l} = 0.922 \int_{x_0}^{x_1} dx + 0.195 \int_{x_1}^{x_2} dx \qquad \text{for } n = 2.$$

where $x_0 = 0$, $x_1 = 0.754$, $x_2 = 1.734$

$$\bar{l} = 0.9798 \int_{x_0}^{x_1} dx + 0.6188 \int_{x_1}^{x_2} dx + 0.1386 \int_{x_2}^{x_3} dx + 0.0051 \int_{x_3}^{x_4} dx \qquad \text{for } n = 4$$

where $x_0 = 0$, $x_1 = 0.4239$ $x_2 = 1.014$ $x_3 = 1.792$ $x_4 = 2.640$

$$\bar{l} = 0.99200 \int_{x_0}^{x_1} dx + 0.81425 \int_{x_1}^{x_2} dx + 0.41032 \int_{x_2}^{x_3} dx + 0.09445 \int_{x_3}^{x_4} dx + 0.00702 \int_{x_4}^{x_5} dx + 0.00008 \int_{x_5}^{x_6} dx \qquad \text{for } n = 6$$

where $x_0 = 0$ $x_1 = 0.27779$ $x_2 = 0.68991$ $x_3 = 1.2090$ $x_4 = 1.8138$ $x_5 = 2.5104$ $x_6 = 3.3556$.

Greater detail on the development of such formulas and their utility will be given in a subsequent paper.

5. References

[1] Hildebrand, F. B., Introduction to Numerical Analysis, p. 319 (Mc-Graw-Hill Book Co., Inc., New York, N.Y. 1956).

[2] Ezrohi. I. A., General Forms of the Remainder Terms of Linear Formulas in Multidimensional Approximate Analysis I and II. Math Sbornik **38** (80) p. 389; Math Rev. **18**, 33. Math Sbornik **43** (85) p. 9; Math Rev. **19**, 1199.

[3] Hammer, P. C., Numerical Evaluation of Multiple Integrals on Numerical Approximation, p. 99, ed. R. E. Langer, University of Wisconsin (1959).

[4] Remez, E. I., On Certain Classes of Linear Functionals in the Spaces C_p and on the Remainder Term in Formulas of Approximate Analysis I and II. Trudy In-Ta Matem Akad, Nauk, Ukr. S.S.R.3, p. 21. Trudy In-Ta Matem, Akad, Nauk, Ukr. S.S.R.4, p. 47, Math Rev **2**, 195.

[5] Sard, A., Function spaces and approximation, Amer. Math. Soc. Numerical Analysis Proc. Symp. Appl. Math **6**, 177.

[6] Day, M. M., Normed Linear Spaces (Springer, Berlin, 1958).

(Paper 70B–173)

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematics and Mathematical Physics
Vol. 70B, No. 2, April–June 1966

Treatment of Outliers in Samples of Size Three*

F. J. Anscombe[1] and Bruce A. Barron[2]

(February 10, 1966)

A reading that is a long way from most of the others in a series of replicate determinations is called an outlier. A particular procedure for rejecting outliers, and also a particular procedure for modifying outliers, are considered for samples of size three, supposed drawn from a common normal population except that one of the three readings may have an added bias. Numerical results are given illustrating the effects of the procedures on estimation of the location parameter. The calculations support a tentative general conclusion that estimation by least squares should usually be tempered by successive application of both a rejection rule and a modification rule.

Key Words: Statistics, outliers, residuals, estimation, robustness, least squares.

1. Introduction

In a situation where one or more parameters are to be estimated by the method of least squares, each observation is regarded as a given linear combination of the parameters plus a random observation error. When the parameters have been estimated, for every observed value a corresponding fitted value can be calculated; the difference between the observed and the fitted value is the residual. Any observed value for which the residual is much larger in magnitude than most of the other residuals is called an outlier.

It has often been suggested that outliers should be treated differently from other observations. Three ways of treating them are

(i) retain the outliers as they stand, giving all observations equal weight;

(ii) reject the outliers, which means giving them zero weight;

(iii) retain the outliers with reduced weight—this is equivalent to modifying the outliers so that they become less different from the other observed values, and then giving them full weight.

This study deals with the effect of using a particular rejection procedure, or alternatively a particular modification procedure, for outliers in samples of size three. The three readings are assumed to be random independent observations drawn from a normal parent population, except that one of the readings may have an added bias. Our object is to estimate the mean of the normal population.

To suppose that some readings are all drawn from a common normal population, except that one has an added bias, may seem an implausible way to represent reality, but consideration of this situation throws useful light on the outlier problem, at less computational expense than some other schemes.

A sample of size three is the smallest for which a study of rejection or modification of outliers, with generation of precise numerical results, is not trivial. The results are of direct interest because chemical determinations are often made in triplicate. Moreover, they provide a check on approximate results and conjectures relating to larger samples.

Lieblein [6] studied the effect of regularly discarding the most discrepant reading from a sample of size three and using the mean of the closest pair as estimate of the population mean. He found the variance of this estimate in various circumstances. Our investigation is similar in spirit to his, though there is no overlap in results.

Dixon [3] was perhaps the first to distinguish clearly two general problems concerning outliers: (a) the problem of identifying a "significant" outlier, in order to infer that something has gone wrong with the experimental procedure, or possibly to explore the outlier as an unusual occurrence of interest; and (b) the problem of obtaining a procedure of analysis not appreciably affected by the presence of abnormal observations. He pointed out that the second problem was important in the estimation of parameters in situations where unavoidable occasional contamination occurred. Using mean squared error as the basis of comparison, he examined several estimates of the population mean (sample mean, median, and mean after application of various rejection rules) under various assumptions of contaminated sampling. Samples of size 5 and 15 were considered, for which an attempt was made to formulate a recommended procedure for processing data for outliers.

Having unfortunately overlooked this work by Dixon, one of the present authors (Anscombe [1][3]) independently made more sweeping suggestions in the same direction: choice of an outlier rejection criterion could often appropriately be based on consideration of its effect on the mean squared error of estimates of the parameters of interest in a least squares analysis,

*Invited paper. Prepared in connection with research at Yale University supported by the Army, Navy, Air Force and NASA under a contract administered by the Office of Naval Research, task NR 042-242, contract Nonr 609(52).

[1] Yale University.
[2] Rockefeller University, New York 21, N.Y.

[3] Figures in brackets indicate the literature references at the end of this paper.

rather than on the traditional rate of rejection. The percentage increase in variance of estimation errors due to using the rule, when in fact all observations came from a homogeneous normal source, would be an appropriate measure of the cost or premium of the procedure; and the reduction in mean squared error when spurious readings were present would measure the protection given by the procedure.

Jeffreys [5] forcefully attacked the use of any outlier rejection rule on several grounds, one being that the resulting estimate of the population mean was a discontinuous function of the observations. He and others, notably Tukey [8] and Huber [4], have made suggestions for assigning reduced but not zero weight to outliers, the weight being a continuous function of the magnitude of the residual. The modification rule considered below is of Huber's type.

With these previous studies in mind, we now formulate procedures for treatment of outliers (in sec. 2) and consider their effectiveness (in secs. 3 and 4), for samples of any size. Then in section 5 our computations for samples of size three are presented and discussed. Tentative general conclusions are drawn in section 6. Some notes on the computations appear in section 7.

2. Definition of Estimation Procedures

Suppose we are given some observations $y_1, y_2, \ldots, y_n$, each of which is a determination or estimate of a common "true" value μ. We wish to combine the observations to form a single improved estimate of μ (or otherwise make inferences about μ).

It is convenient to define the sample mean $\bar{y}$, the residuals z_i $(i = 1, 2, \ldots, n)$ and the number ν of residual degrees of freedom by

$$n\bar{y} = \sum_i y_i, \qquad z_i = y_i - \bar{y}, \qquad \nu = n - 1. \tag{1}$$

The custom in this situation is to hope that (near enough) the y's are realizations of independent random variables each having the same normal distribution with mean μ.

If this hope were believed to be accurately fulfilled, the estimation problem would be well defined and easy. If the variance of the common normal distribution were supposed known, the sufficient statistics $\bar{y}$ and n would constitute a complete summary of the data; and if the variance were not known, the sufficient statistics $\bar{y}$, n, and $\Sigma_i z_i^2$ would be a complete summary. In either case, we could regard $\bar{y}$ as estimating μ, with the other statistics ancillary. As is well known, $\bar{y}$ is the value for μ at which the sum of squares

$$\Sigma_i (y_i - \mu)^2 \tag{2}$$

is minimized.

But ordinarily it is unreasonable to suppose that the hoped-for property of the y's is accurately true. If we think in terms of a single estimate of μ, $\bar{y}$ is not necessarily the best to choose. In particular, we should usually bear in mind that the observations may have a propensity towards outliers. Two alternative theoretical descriptions of an outlier phenomenon are (i) some of the observations are affected by a gross error or mistake, which adds a bias onto the reading that would otherwise be obtained, (ii) the distribution of deviations of the observations from μ is not normal, but has longer tails, like a logistic distribution, for example. (Further theoretical descriptions are easily invented.) We therefore consider how to define a function $\hat{\mu}$ of the observations that may possibly estimate μ satisfactorily when some kind of outlier phenomenon is present. The difficulty here arises from our reluctance to specify firmly the distribution of the observations in terms of a very few parameters.

The traditional way of treating outliers is to reject them according to some rule and then let $\hat{\mu}$ be the average of the remaining observations. We here consider the following rule, as an example. First a critical size K for a residual is chosen $(K > 0)$. Then the rule is

Rejection rule. Let M be a value of i for which $|z_i|$ is greatest. (M may be expected to be unique if $n \geq 3$ and if the observations are recorded with high precision.) If $n = 2$, or if $n \geq 3$ and also $|z_M| \leq K$, retain all observations and quote $\bar{y}$ as the estimate of μ. If $n \geq 3$ and also $|z_M| > K$, reject y_M from the sample and act as though the remaining $n - 1$ observations were the whole sample. With the observations relabeled and n and z's redefined, go back to the start of this rule.

If the initial sample size is 2, the rule sets $\hat{\mu}$ equal to the simple mean $\bar{y}$ in any case. If the initial sample size is 3, the rule leads *either* to retention of all three observations with equal weight (if $|z_M| \leq K$), so that $\hat{\mu} = \bar{y}$, *or* to rejection of just one observation, so that $\hat{\mu}$ is the average of the other two observations. If the initial sample size n exceeds 3, the rule leads conceivably to rejection of any number of observations from 0 to $n - 2$, inclusive.

To implement the suggestion that outliers ought to be given reduced but not zero weight, we also consider the following rule, which seems to be computationally the simplest possible such rule. A critical size K for a residual is chosen $(K > 0)$. Then the rule is

Modification rule. Choose as $\hat{\mu}$ a value for μ at which

$$\Sigma_{(1)} (y_i - \mu)^2 + \Sigma_{(2)} K\{2|y_i - \mu| - K\} \tag{3}$$

is minimized, where $\Sigma_{(1)}$ means summation over those values of i for which $|y_i - \mu| \leq K$ and $\Sigma_{(2)}$ means summation over the remaining values of i. ($\hat{\mu}$ is unique provided there is at least one value of i for which $|y_i - \hat{\mu}| < K$.)

This rule may be alternatively expressed by saying that $\hat{\mu}$ is chosen to minimize the sum of squares (2),

but under a condition that some observations are modified if necessary so that no residual exceeds K in magnitude. Specifically, each observation y_i such that $|y_i-\hat{\mu}|>K$ is modified to a value y_i^* such that $y_i^*-\hat{\mu}$ has the same sign as $y_i-\hat{\mu}$ but $|y_i^*-\hat{\mu}|=K$. Which observations are to be modified (or in the previous language, which observations are to be included in the second summation $\Sigma_{(2)}$) must in general be discovered in several steps of trial and error, a task of quadratic programming. (It has been considered, for general regression analysis, by Sand [7].)

When $n=2$, we may always set $\hat{\mu}=\bar{y}$. This is the unique possibility for $\hat{\mu}$ if the two observations are spaced not more than $2K$ apart. Otherwise $\hat{\mu}$ may be chosen anywhere in an interval of width $|y_1-y_2|-2K$, centered at $\bar{y}$.

When $n=3$, let $y_{(1)}$, $y_{(2)}$, $y_{(3)}$ denote the three observations, rearranged in ascending order of magnitude. Then $\hat{\mu}$ is determined as follows:

(i) If $\bar{y}-y_{(1)}$ and $y_{(3)}-\bar{y}$ are both not greater than K, no observation is modified and $\hat{\mu}=\bar{y}$.

(ii) If $y_{(2)}-y_{(1)}$ and $y_{(3)}-y_{(2)}$ both exceed K, $y_{(1)}$ and $y_{(3)}$ are both modified and $\hat{\mu}=y_{(2)}$, the median.

(iii) Otherwise, either $y_{(1)}$ or $y_{(3)}$, but not both, is modified. If, for example, $y_{(3)}$ is modified (because $y_{(3)}-\bar{y}>K$ and $y_{(3)}-y_{(2)}>K>y_{(2)}-y_{(1)}$), $\hat{\mu}$ is defined by

$$2\hat{\mu}=y_{(1)}+y_{(2)}+K.$$

$\hat{\mu}$ lies between the mean $\bar{y}$ and the median $y_{(2)}$. (In case (ii), the modified observations are $y_{(1)}^*=y_{(2)}-K$, $y_{(3)}^*=y_{(2)}+K$. In case (iii), if $y_{(3)}$ is modified, $y_{(3)}^*=\hat{\mu}+K$ and $3\hat{\mu}=y_{(1)}+y_{(2)}+y_{(3)}^*$.)

3. Distribution Assumption

The above rules yield estimates $\hat{\mu}$ of μ that are desensitized to outliers and may therefore be preferred to $\bar{y}$. For each rule, $\hat{\mu}$ is a function of the n observations and of K. We could distinguish the two functions with a suffix, but that will be unnecessary because we shall always make clear which rule is under discussion.

In order to assess the effectiveness of the rules, seeing how the effectiveness of each varies with K and how one rule compares with the other, we need to specify the true statistical properties of the observations. In this paper we suppose that the observations have the hoped-for property exactly, except that possibly *one* observation has an added bias. That is, we make the

Assumption: the y's are realizations of independent random variables each normally distributed with the same variance σ^2 and with these expectations:

$$E(y_i)=\mu\ (i=1,2,\ldots,n-1), \qquad E(y_n)=\mu+b\sigma. \tag{4}$$

We here take the liberty of using y_i both as the name of the random variable corresponding to the ith observation and as the name of that observation.

We shall be interested in the ratio of K to σ, which we denote by C, thus:

$$K=C\sigma. \tag{5}$$

We shall take expectations with respect to the above random variables, for fixed μ, σ, C, and b. Having σ and C fixed implies that K is fixed and therefore not determined by the observations themselves (as it would be, for example, if K were chosen to be equal to a given multiple of the sample standard deviation).

An alternative distribution assumption that would be interesting, but is not considered in this paper, would be that the observations were independently drawn from a common nonnormal distribution with mean μ, such as a logistic distribution.

4. Formulas

For better or worse, we shall assess the effectiveness of the two rules for treating outliers through the mean squared error of the sampling distribution of $\hat{\mu}$, under the above distribution assumption. Hopefully, when $b=0$, we shall find that the variance (which is also the mean squared error) of $\hat{\mu}$ is little larger than that of $\bar{y}$, namely σ^2/n, but when b is large $E(\hat{\mu}-\mu)^2$ will be smaller than

$$E(\bar{y}-\mu)^2=(\sigma^2/n)\{1+(b^2/n)\}. \tag{6}$$

To determine $E(\hat{\mu}-\mu)^2$ precisely, under the above distribution assumption, is a formidable task even when n is as small as 3. If we define an orthogonal linear transformation (Helmert transformation) of the y's, so that the new variables are $\bar{y}\sqrt{n}$, x_1, x_2, . . ., x_{n-1}, say, these variables are independently normally distributed with the same variance σ^2. We may write

$$\hat{\mu}-\mu=\{\bar{y}-\mu-(b\sigma/n)\}+U\sigma, \tag{7}$$

where U is a function of the x's but not of $\bar{y}$. Hence

$$E(\hat{\mu}-\mu)^2=(\sigma^2/n)+\sigma^2E(U^2),$$

or

$$(n/\sigma^2)E(\hat{\mu}-\mu)^2=1+nE(U^2). \tag{8}$$

$E(U^2)$ can be expressed as an $(n-1)$-dimensional integral. The form of the integrand depends on which of various linear inequalities among the x's are satisfied, so that the region of integration is divided into many zones, in each of which the integrand has a simple expression, different from zone to zone.

The main purpose of this paper is to present results of the calculation of $E(\hat{\mu}-\mu)^2$ when $n=3$. Values of $(3/\sigma^2)E(\hat{\mu}-\mu)^2$ are shown for an assortment of values

of C and b in table 1 (for the rejection rule) and table 2 (modification rule).

The case $n=3$ is important in its own right, and moreover may give some indication of the behavior of $E(\hat{\mu}-\mu)^2$ for larger values of n. For the latter purpose, it is useful to have some information about limiting values and approximations. These are now summarized.

Rejection rule. When $b=0$, the following approximate expression for the variance (mean squared error) of μ has been given [1]:

$$(n/\sigma^2)\ \mathrm{var}(\hat{\mu}) \doteq 1+(n/\nu)\{2t_a\varphi(t_a)+\alpha\}, \qquad (9)$$

where

$$t_a=C\sqrt{n/\nu}, \qquad \alpha=2\Phi(-t_a)$$

and the functions Φ and φ are defined thus:

$$\Phi(t)=\int_{-\infty}^{t}\varphi(u)du, \qquad \varphi(u)=e^{-u^2/2}/\sqrt{2\pi}.$$

This result is asymptotically correct as $C\to\infty$ with n and ν fixed, and may be expected to be fairly good if C is somewhat greater than 2.

A more easily calculated formula, alternative to (9) when $b=0$, can be obtained, similar to one given by Anscombe and Tukey [2]:

$$(n/\sigma^2)\ \mathrm{var}(\hat{\mu}) \doteq 1+(n/\nu)\Phi(-N), \qquad (10)$$

where N is defined in terms of the above t_a by

$$t_a=1.40+0.85\,N.$$

When $b\to\infty$ with C fixed, rejection of the "bad" observation y_n becomes certain, and if no further rejection occurred we should have for the variance (mean squared error) of $\hat{\mu}$

$$(n/\sigma^2)\ \mathrm{var}(\hat{\mu})\to 1+(1/\nu). \qquad (11)$$

This is accurately true when $n=3$, because no further rejections are allowed. For $n\geq 4$, the right side of (11) should be increased to allow for the effect of possible further rejections. A lower bound for $E(\hat{\mu}-\mu)^2$ when b is large but not infinite has been given ([1], eq (6.3)), but appears from the present calculations to be a very poor approximation.[4]

Modification rule. When $b=0$, the result for the modification rule corresponding to (9) above for the rejection rule is

$$(n/\sigma^2)\ \mathrm{var}(\hat{\mu}) \doteq 1+(n/\nu)\{(1+t_a^2)\alpha-2t_a\varphi(t_a)\}, \qquad (12)$$

t_a and α being defined as before. This formula may be expected to be less helpful than (9). Both formulas are derived assuming C to be so large that few observations are rejected or modified (as the case may be) and the negative correlation between residuals within a sample is unimportant. But the values of C that are of practical interest are smaller for the modification rule than for the rejection rule.

When $b\to\infty$ with C fixed, modification of the "bad" observation y_n becomes certain, and if no further modification occurred we should have

$$(n/\sigma^2)E(\hat{\mu}-\mu)^2\to 1+(1/\nu)+(nC^2/\nu^2). \qquad (13)$$

In fact, however, other observations may be modified, and because of the positive bias resulting from y_n the tendency will be for low readings to be modified upwards rather than for high readings to be modified downwards. It follows that the right side of (13) is too low. For $n=3$, $\nu=2$, it is not hard to show that the correct result is

$$(3/\sigma^2)E(\hat{\mu}-\mu)^2\to\frac{3}{2}+\frac{3C^2}{4}+\frac{3C}{\sqrt{2}}\varphi\left(\frac{C}{\sqrt{2}}\right)+3\left(1-\frac{C^2}{2}\right)\Phi\left(-\frac{C}{\sqrt{2}}\right). \qquad (14)$$

Note. Although in section 2 we explicitly mentioned only the possibility that the y's were all determinations of the same location parameter μ, much of what has been said can be adapted to regression analysis, μ being replaced by a linear function of parameters β_r. Formulas (6), (9), (10), (11), (12), and (13) are valid with the following amendment and reinterpretation. The y's are observations in a factorial experiment with n experimental units (n being even) and an orthogonal design matrix. We focus attention on one particular two-level factor; this appears $n/2$ times at its upper level, $n/2$ times at its lower level. Let β_1 stand for one half of the response to this factor, so that $2\beta_1$ is the change in the expectation of an observation caused by changing the level of the factor from lower to upper; let b_1 denote the usual estimate of β_1 (total of observations for which the factor is at the upper level minus total of other observations, divided by n); and let $\hat{\beta}_1$ denote the estimate of β_1 yielded by the rejection or modification rule (as the case may be). Let $\{z_i\}$ be the residuals and ν the number of residual degrees of freedom after the estimation of all factor effects by least squares, and let the $n\times n$ matrix (q_{ij}) be defined by

$$z_i=\sum_j q_{ij}y_j.$$

We assume that for all i and j

$$q_{ii}=\nu/n, \qquad |q_{ij}|<\nu/n \qquad (i\neq j).$$

[4] The b-values in table 3 of [1] are presumably substantially too low, but possibly the remarks based on them are correct.

On the left sides of the above mentioned formulas, replace μ, $\bar{y}$, and $\hat{\mu}$ by β_1, b_1, and $\hat{\beta}_1$.

5. Results of Computation

Tables 1 and 2 present the mean squared error of $\hat{\mu}$ when $n=3$. The nine values for C are the "round" numbers 1, 1.5, 2, 3, and ∞, and also the values for which the entry in the first row (for $b=0$) is 1.04, 1.02, 1.01, and 1.005. The last column ($C=\infty$) refers to use of the unadjusted mean, $\bar{y}$, as the estimate of μ; the values are given by formula (6). Various values for the bias factor b are shown. In the last line of each table, except for the entry in the last column ($C=\infty$), the entries are exactly equal (to the number of decimal places shown) to the limiting values as $b\to\infty$ given in formulas (11) and (14).

The percentage increase in sampling variance resulting from use of $\hat{\mu}$ instead of $\bar{y}$, when all the observations have a common normal distribution (the hoped-for property), may be termed the premium charged by the rule. The premium may be read from the first line of tables 1 and 2 (for $b=0$) by subtracting the initial 1 and multiplying by 100.

In figure 1 mean squared error is graphed against b for (i) the unadjusted mean $\bar{y}$, (ii) $\hat{\mu}$ given by the rejection rule with 2 percent premium, (iii) $\hat{\mu}$ given by the modification rule, also with 2 percent premium.

Table 3 compares approximations (9), (10), and (12) with the correct values. (For (9) see also table 4 of [1].)

So far so good. The burning question that faces us is what do these computations show concerning the relative merits of the two methods of treating outliers, and if we decide to use either one, how should

TABLE 1. *Values of* $(3/\sigma^2)E(\hat{\mu}-\mu)^2$ *for the rejection rule*

	$C=1.00$	1.50	2.00	2.46003	2.66184	2.84623	3.00	3.01724	∞
$b=0.00$	1.7318	1.4116	1.1496	1.0400	1.0200	1.0100	1.0054	1.0050	1.0000
.25	1.7731	1.4510	1.1812	1.0650	1.0433	1.0322	1.0270	1.0266	1.0208
.50	1.8931	1.5664	1.2753	1.1403	1.1133	1.0991	1.0921	1.0916	1.0833
1.00	2.3163	1.9896	1.6404	1.4422	1.3956	1.3688	1.3546	1.3534	1.3333
1.50	2.8488	2.5649	2.1969	1.9395	1.8682	1.8229	1.7969	1.7946	1.7500
2.00	3.3185	3.1297	2.8401	2.5914	2.5097	2.4522	2.4161	2.4126	2.3333
3.00	3.6602	3.6782	3.7634	3.8852	3.9340	3.9698	3.9917	3.9936	4.0000
4.00	3.2476	3.3066	3.5722	4.1362	4.4702	4.7967	5.0682	5.0980	6.3333
6.00	2.0323	2.0353	2.0674	2.2339	2.4143	2.6761	2.9854	3.0259	13.0000
8.00	1.5712	1.5712	1.5712	1.5737	1.5780	1.5872	1.6025	1.6048	22.3333
10.00	1.5045	1.5045	1.5045	1.5045	1.5045	1.5045	1.5045	1.5045	34.3333
12.00	1.5001	1.5001	1.5001	1.5001	1.5001	1.5001	1.5001	1.5001	49.0000
15.00	1.5000	1.5000	1.5000	1.5000	1.5000	1.5000	1.5000	1.5000	76.0000

TABLE 2. *Values of* $(3/\sigma^2)E(\hat{\mu}-\mu)^2$ *for the modification rule*

	$C=1.00$	1.29420	1.50	1.52486	1.73307	1.92458	2.00	3.00	∞
$b=0.00$	1.0860	1.0400	1.0216	1.0200	1.0100	1.0050	1.0038	1.00004	1.0000
.25	1.1106	1.0631	1.0439	1.0422	1.0316	1.0263	1.0249	1.0209	1.0208
.50	1.1830	1.1315	1.1102	1.1082	1.0962	1.0899	1.0883	1.0834	1.0833
1.00	1.4512	1.3909	1.3651	1.3627	1.3480	1.3404	1.3385	1.3333	1.3333
1.50	1.8295	1.7743	1.7532	1.7516	1.7424	1.7400	1.7401	1.7487	1.7500
2.00	2.2380	2.2156	2.2189	2.2202	2.2354	2.2540	2.2616	2.3256	2.3333
3.00	2.8859	2.9970	3.1075	3.1223	3.2546	3.3830	3.4333	3.9014	4.0000
4.00	3.1789	3.4116	3.6342	3.6642	3.9389	4.2212	4.3376	5.7419	6.3333
6.00	3.2675	3.5619	3.8520	3.8920	4.2701	4.6861	4.8677	8.0425	13.0000
8.00	3.2687	3.5645	3.8566	3.8970	4.2789	4.7014	4.8867	8.3350	22.3333
10.00	3.2687	3.5646	3.8566	3.8970	4.2790	4.7014	4.8867	8.3396	34.3333

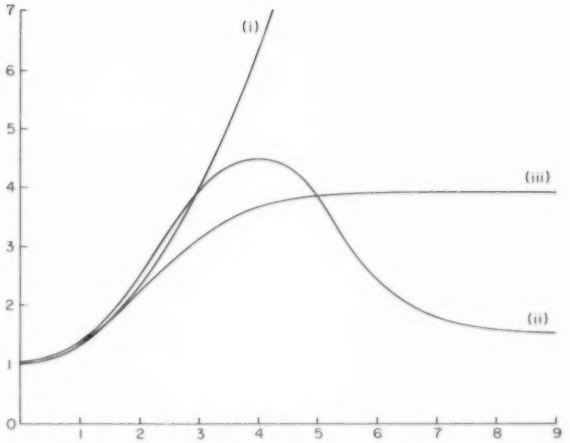

FIGURE 1. *Curves showing* $(3/\sigma^2)E(\hat{\mu}-\mu)^2$ *as a function of* b.

K be chosen? No set of calculations such as ours can settle the matter beyond dispute, because we do not know that reality is well represented by the distribution assumption that we have used, nor by any other distribution assumption that we might have used instead. However, in the light of such theoretical knowledge as we have, the calculations do seem to support some clear-cut conclusions that may have general validity in regression analysis.

TABLE 3. *Approximations to* $(3/\sigma^2)$ *var* $(\hat{\mu})$ *when* $b=0$

	$C=1.00$	1.50	2.00	3.00
Rejection rule:				
Correct Value	1.7318	1.4116	1.1496	1.0054
Approximation (9)	2.0234	1.5060	1.1674	1.0055
Approximation (10)	1.8725	1.4553	1.1627	1.0056
Modification rule:				
Correct value	1.0860	1.0216	1.0038	1.00004
Approximation (12)	1.1351	1.0277	1.0043	1.00004

We see from the tables that if b is small, in the range 0 to 1.5, both rules give estimates inferior to the unadjusted $\bar{y}$. If b is in a middle range, roughly from 2 to 4, the modification rule fares best. If b is above 5 or 6, the rejection rule is much better than the modification rule, which in turn is very much better than $\bar{y}$. These comparisons hold fairly consistently, when we compare a rejection rule with a modification rule *either* having the same premium (as in fig. 1) *or* having the same value for C. Thus which type of rule is to be preferred depends on how large we expect b will be (insofar as our distribution assumption can be accepted as a description of the facts).

Now we can distinguish two quite different processes that lead to outliers in a series of readings. On the one hand there may be mistakes or failures to do what

is intended—instrumental failures, errors in transcription or in arithmetic, mixed-up records, etc. A reading affected by an accident of this sort may easily lie a great distance from other readings. Therefore if we wish to guard against such gross errors, it is reasonable to choose a rejection rule. In practice, most observers discard extremely aberrant readings as obviously wrong, without any explicit rule, provided that they actually examine the readings. More and more nowadays the output of instruments is fed directly to a computer for processing, and then it is important that proper provision should be made for intercepting gross errors.

On the other hand, outliers may arise in good observations when no blunder or failure has occurred. The normal law of errors beloved of statistical theorists is not a law of nature, and observational errors do not have to conform to it. Probably many actual error distributions have somewhat longer tails than the normal. Jeffreys [5] reports some investigations of errors in astronomical readings, and suggests that a homogeneous series of readings by one observer may be expected to follow a Pearson Type VII distribution, having the same shape as a Student distribution with 7 deg of freedom. Tukey has pointed out (privately) that this distribution has nearly the same shape as a logistic distribution—the difference could hardly be detected empirically. In view of the distribution assumption of the present paper, it is interesting to note that the Student distribution with 7 deg of freedom is even more closely approximated by the distribution of the sum of two independent random variables, $X+Y$, where X is normally distributed and Y has chance 0.95 of being equal to 0 and chance 0.05 of being equal in magnitude to three times the standard deviation of X (positive or negative with equal chances).[5] This suggests that, to represent Jeffreys's type of long-tailed distribution of errors with the distribution assumption of this paper, we should regard b as taking the values 0 and 3 with something like a 6:1 frequency ratio. (Our distribution assumption cannot exactly represent samples of size 3 from the distribution of $X+Y$, because in a few such samples (less than 1 %) there would be more than one non-zero Y-value, and our calculations do not apply.) For these values of b, our tables indicate that the modification type of rule should be used.

This finding fits well with the consideration of maximum likelihood estimation of μ when the errors have a long-tailed distribution (see [2], sec. 8). In particular, maximum likelihood estimation of the location parameter of a logistic distribution is closely approximated by our modification rule, when K is about 1.1 times the true standard deviation of the logistic distribution, or about 1.25 times a pseudo standard deviation estimated from the slope of the middle part of the cumulative frequency curve plotted on "probability" graph paper (this being the sort of estimate of σ that we might make from past records if we believed that the error distribution was normal except for some outliers).

Thus our calculations support the following general conclusions which are closely in line with suggestions made by Tukey [8].

6. Tentative Conclusions

Whenever we think of applying the method of least squares to some readings in order to estimate a parameter or parameters of location, we shall do well to recognize the two possibilities that (i) occasionally a reading may be "bad", grossly in error and useless for the estimation purpose at hand (though possibly interesting for other reasons), and (ii) the "good" readings may have a somewhat longer-tailed distribution than the normal. In view of these possibilities (especially when the statistical analysis is computerized), it will be advisable to use first a rejection rule and then a modification rule. The rejection rule should have K so large that it will almost never reject "good" observations, but will protect against really "bad" ones. The modification rule will have a lower value for K and will aim to yield good estimates if the error distribution does not greatly differ from a normal or a logistic distribution. Actually the choice of K for the modification rule is likely to depend not only on considerations of efficiency of estimation but also on speed in computation. The smaller K is, the more iterations may be needed to carry out the modification procedure. It may therefore be wise to choose K so that not more than a few percent of readings (on the average) will be modified.

How to estimate from the data the precision of estimates obtained through the modification rule seems not to be well understood at present. But one thing at a time! (For a sample of size 3 such estimation is ludicrous anyway; hence the assumption in our calculations that σ was known.)

Of course when large collections of similar data are available for study, it is possible to investigate their statistical properties and adjust the estimation procedures accordingly. But in the absence of a special study it would be good routine practice always to temper the method of least squares by the combined rejection-modification procedure just outlined.

7. Notes on the Computation

We may set

$$x_1 = \frac{y_1 - y_2}{\sqrt{2}} = \frac{z_1 - z_2}{\sqrt{2}}$$

$$x_2 = \frac{2y_3 - y_1 - y_2}{\sqrt{6}} = z_3 \sqrt{\frac{3}{2}}.$$

[5] The middle ordinate of the density function, multiplied by the standard deviation, makes a good index of shape. For (i) the Student distribution, (ii) the logistic, (iii) the distribution of $X+Y$, as specified, this index is approximately (i) 0.4555, (ii) 0.4534, (iii) 0.4566. Fisher's shape coefficient γ_2 (fourth cumulant divided by squared variance) comes out: (i) 2, (ii) 1.2, (iii) 1.637.

Under the distribution assumption, x_1 and x_2 are independently normally distributed with means 0 and $b\sigma\sqrt{2/3}$ and with the same variance σ^2. Expressing U in terms of x_1 and x_2, we evaluate $E(U^2)$ by integration over the (x_1, x_2)-plane. The region of integration is divided into zones, as sketched in figure 2. The inner zone is a hexagon bounded by the three pairs of parallel lines,

$$z_1 = \pm C\sigma, \qquad z_2 = \pm C\sigma, \qquad z_3 = \pm C\sigma.$$

For the rejection rule, the region outside the hexagon is divided into six zones, corresponding to the six possible combinations of three values for M and two signs for z_M. For the modification rule the region outside the hexagon is divided into twelve zones, corresponding to the above six possibilities concerning z_M when y_M is the only modified observation, plus six possibilities for choosing a pair of observations to be modified, one of the residuals being positive and the other negative.

Inside the hexagon U has the constant value $b/3$. In each of the other zones U is a linear function of x_1 and x_2. For example, the zone labeled A in the rejection-rule part of figure 2 is defined by the properties:

$$M = 3, \qquad z_3 > C\sigma,$$

and in this zone we have

$$U = \frac{b}{3} - \frac{x_2}{\sigma\sqrt{6}}.$$

The zone labeled B in the modification-rule part of figure 2 is defined by the properties:

$$M = 3, \qquad z_3 > C\sigma, \qquad \text{only } y_3 \text{ is modified,}$$

and in this zone we have

$$U = \frac{b}{3} + \frac{C}{2} - \frac{x_2}{\sigma\sqrt{6}}.$$

The zone labeled C is defined by the properties:

$$y_2 \text{ and } y_3 \text{ are modified,} \quad y_3 - y_1 > C\sigma, \quad y_1 - y_2 > C\sigma,$$

and in this zone we have

$$U = \frac{b}{3} + \frac{x_1\sqrt{3} - x_2}{\sigma\sqrt{6}}.$$

In all the above it is convenient and permissible to set $\sigma = 1$.

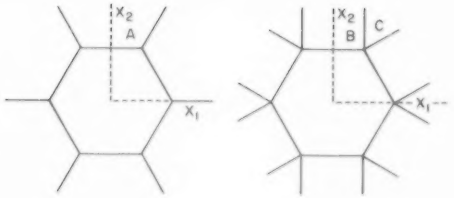

FIGURE 2. *Zones of integration.*
The diagram on the left is for the rejection rule, that on the right for the modification rule.

In principle it is possible to evaluate the double integral over each zone by expressing it as a single integral in terms of the normal integral and density functions and then using single numerical quadrature. But because that would involve much tedious detail in rotating axes, it seemed cheaper to use double numerical quadrature, integrating first for x_2 and then for x_1 by Simpson's rule. Integration was carried out over a square area of the plane, so that x_1 and x_2 ranged 5.5σ above and below their means. The integrand is well behaved within each zone but is singular on every boundary between zones. A not quite uniform grid of points was used for evaluating the integrand, so that boundaries were always encountered as end points of individual applications of Simpson's rule, never as interior points. The interval width in x_1 and x_2 of 0.10σ (or less as needed to hit the boundaries cleanly) was found satisfactory. The program was tested by finding the expectation of simple random variables whose form did not change from zone to zone. The work was done at the Yale Computer Center (IBM 7040–7094 DCS).

8. References

[1] Anscombe, F. J., Rejection of outliers, Technometrics **2**, 123–147 (1960).

[2] Anscombe, F. J. and Tukey, John W., The examination and analysis of residuals, Technometrics **5**, 141–160 (1963).

[3] Dixon, W. J., Processing data for outliers, Biometrics **9**, 74–89 (1953).

[4] Huber, Peter J., Robust estimation of a location parameter, Annals of Mathematical Statistics **35**, 73–101 (1964).

[5] Jeffreys, Harold, Theory of Probability, Oxford, Clarendon Press (1939, 1948, 1961). See sections 4.4 (all editions) and 5.7 (second and third editions, based on 5.77 in the first edition).

[6] Lieblein, Julius, Properties of certain statistics involving the closest pair in a sample of three observations, J. Res. NBS **48**, 255–268 (1952) RP2311.

[7] Sand, Francis, Investigations in residual analysis and a modification of the least-squares method for multiple regression, Ph. D. thesis, Princeton University (1963).

[8] Tukey, John W., The future of data analysis, Annals of Mathematical Statistics **33**, 1–67 (1962).

(Paper 70B2–174)

JOURNAL OF RESEARCH of the National Bureau of Standards – B. Mathematics and Mathematical Physics
Vol. 70B, No. 2, April–June 1966

A Note on Contaminated Samples of Size Three

T. A. Willke*

(February 25, 1966)

Estimation of the mean and standard deviation using the closest two of three observations in a sample from a normal population with contamination by slippage of the mean is investigated by a sampling study. Lieblein's results, which indicated that the use of these statistics is not advisable for noncontaminated samples, are borne out by this study for contaminated samples as well.

Key Words: Outliers, contaminated samples, robust estimates, best two of three.

1. Introduction

In the physical sciences samples of only three measurements of a quantity are not uncommon, and estimation of the actual value of the quantity from these few measurements poses some difficult problems. If it is known that all of the measurements are good, that is, that they are measurements of the same quantity and that they contain no blunders or gross errors, then the sample mean has no serious competitor as an estimate of the true mean for measurement data which are approximately normally distributed.

Quite often, though, there is a definite possibility that one or more of the measurements contain an error which is not just due to the uncertainties of the measurement process, but which results from a slip in the procedure, a failure of some component of the measurement apparatus, a misread dial, etc. Such a measurement is called a contaminant and sometimes, depending on the purpose of the experiment, should be discarded from the sample. Unfortunately, unless the error is very large it is usually difficult to determine whether a measurement is a contaminant or not. The chemistry lab teacher who advises his students to take three measurements and use only the closest two of them in their calculations has recognized this problem and uses this device in an attempt to get robust estimates which are not likely to be as affected by a contaminant as the ordinary estimates are. The main purpose of this paper is to examine how sound this procedure is.

Lieblein [1955] derived distributions of some statistics, especially the mean and the range of the closest two of three independent observations from the same normal distribution, and he discussed their properties as estimators of the mean and the standard deviation of the population. He found them to be inefficient and generally unreliable compared to the mean and the range of all three observations. However, an experimenter would use the closest two of three observations to compute his estimates only if he thought that the sample might be contaminated. Lieblein considered the null case where no contamination exists, hence he has evaluated the penalty one must pay by using these protected estimates when they are not really needed. To complete the picture we must find out how much, if any, the experimenter stands to gain if there is contamination, and thus see how robust these estimates really are. This, of course, depends on how much and what kind of contamination is present, and this note describes the results of a sampling experiment in the important case where the contamination is by slippage of the mean. It is assumed throughout that the standard deviation is not known. If some prior knowledge of the standard deviation is available the contaminants are easier to detect and the treatment of the problem is changed.

2. Estimation of the Mean With Exactly One Contaminant

Let x_1, x_2, x_3, be an independent sample of size three with x_1 and x_2 from a normal distribution with the mean μ and the variance σ^2. Let x_3 be from a normal distribution with the mean $\mu+\delta\sigma$ and variance σ^2. The order statistics for the sample will be denoted $x_{(1)} < x_{(2)} < x_{(3)}$. Let x' and x'' be the closest two of the three observations with $x' < x''$. Then consider the following statistics as estimates of the mean;

$$\bar{x} = (1/3)\sum x_i$$

$$m = x_{(2)}$$

$$y_3 = (1/2)(x' + x'').$$

In particular we are interested in (1) the bias or the difference between the expected value of the statistic and μ, and (2) the root mean square error of the estimate from μ. In the null case, $\delta = 0$, all three esti-

*University of Maryland, College Park, Md.; part time at the National Bureau of Standards.

mates are unbiased and the root mean square errors of $\bar{x}$ and m are known to be

$$\{E[(\bar{x}-\mu)^2]\}^{1/2}=\frac{\sigma}{\sqrt{3}}=0.577\sigma, \text{ and}$$

$$\{E[(m-\mu)^2]\}^{1/2}=0.670\sigma;$$

and of y_3 was found by Lieblein to be

$$\{E[(y_3-\mu)^2]\}^{1/2}=\left(\frac{1}{2}+\frac{\sqrt{3}}{4\pi}\right)^{1/2}\sigma=0.799\sigma.$$

Thus, in the null case, the sample mean is about twice as efficient as y_3. It should be noted that y_3 has a larger standard error than the mean of an uncontaminated sample of size two has (0.707σ), so that when there is no contamination the chemistry student is better off taking just two measurements and averaging them than he is taking three and using the best two of the three.

In the sampling experiment 1,000 samples of size three (containing two uncontaminated values, x_1 and x_2, and one contaminated value, x_3) were taken for each of the values $\delta=0$, 1, 2, 3, 4, and 6, to see how the above estimators performed in nonnull situations. The bias and the root mean square error of these estimates as determined by the sampling experiment are graphed in figure 1. (The results of the sampling experiment agree with the exact values, which are known for $\delta=0$ and for $\bar{x}$, almost to within the accuracy of the graphs. The graphs for the median, m, are exact values calculated from its probability distribution function.)

The three lines in the graphs labeled $\eta=1/3$, $\eta=1/6$ and $\eta=1/11$ correspond to estimates of the mean where either $\bar{x}$ or y_3 is used depending on the spacing of the three measurements as follows. If the spacing between the three measurements is about the same, then there is little evidence of a contaminant and one would want to use $\bar{x}$. However, if one of the three is relatively far removed from the other two, then the natural tendency is to discard it and use the average of the other two, namely y_3. A decision rule for this policy can be formulated as follows. Let

$$u=x''-x'$$

$$\omega=x_{(3)}-x_{(1)}.$$

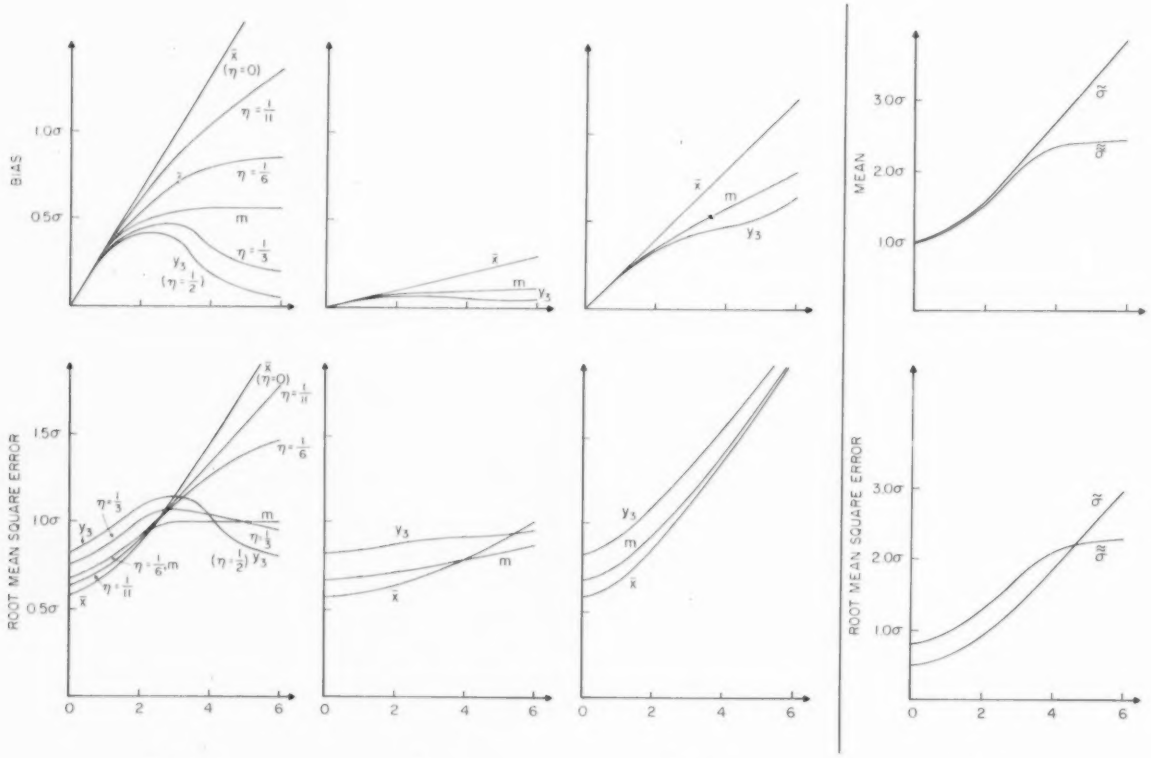

FIGURE 1
Exactly one contaminant

FIGURE 2
5% contamination

FIGURE 3
20% contamination

FIGURE 4
Exactly one contaminant

Biases and root mean square errors for various estimates of the mean.

Means and root mean square errors for two estimates of the standard deviation.

Then, if $\frac{\bar{u}}{\omega} < \eta$, where η is a preassigned constant, use y_3 as the estimate, and if $\frac{\bar{u}}{\omega} \geq \eta$ use $\bar{x}$. For example, suppose η is chosen to be $\frac{1}{11}$, then if the measurement on one end is more than ten times as far from the middle measurement as the one on the other end, y_3 is used; otherwise $\bar{x}$ is used. Notice that $\eta = 0$ corresponds to using $\bar{x}$ always and $\eta = \frac{1}{2}$ corresponds to using y_3 always.

The bias in $\bar{x}$ increases linearly with δ whereas that of y_3 goes to 0 since the two good measurements are almost always used for y_3 when δ is large. For the same reason the bias in the median levels out to 0.564σ, the expected value of the second order statistic in a sample of size two.

The graph of the root mean square error shows that although in the null case y_3 is quite inefficient, it results in a real saving for large values of δ and this fact would seem to support the opinion of the chemistry teacher.

3. Estimation of the Mean With a Random Number of Contaminants

The graphs discussed above can be misleading since they are for a model in which there is known to be exactly one contaminant. In practice the difficult task usually is to decide whether there is a contaminant present. Even in noncontaminated samples the ratio $\frac{u}{\omega}$ can be deceptively small (the probability that $\frac{u}{\omega} \leq \frac{1}{11}$ is about 0.157). Someone who does not fully appreciate the vagaries of small samples can easily be led to believe there is a contaminant present when there are none.

Perhaps a more realistic model would be to assume that any one of the measurements has a certain chance of being contaminated, hence there could be 0, 1, 2, or even 3 contaminants in the sample. If there are two or three contaminants in a sample of three then estimation of the mean is hopeless anyway, but it is possible that the use of y_3 leads to a false sense of security, or does even more damage than $\bar{x}$ or m, particularly when all contaminants are from the same source.

In figures 2 and 3 are graphed the bias and the root mean square error for these estimates when there is a 5 percent and a 20 percent chance respectively that each particular measurement is a contaminant and when this probability is independent of the probability for the other two measurements. The graphs were calculated from the results of the sampling experiment above by the use of binomial probabilities. For this model y_3 loses much of its advantage, especially for the high contamination of 20 percent because there is a reasonable chance that two of the sample values are contaminants and then y_3 exhibits even a larger bias than $\bar{x}$. Moreover, x has a uniformly smaller root mean square error than either y_3 or m has up to $\delta = 6$. This, of course, is true only because in this model all contaminants have their mean displaced in the same direction. If contamination comes from both sides the bias may be eliminated.

The graphs for the optional estimates with $\eta = 1/3$, 1/6, and 1/11 are not given, but they lie midway between the graphs of y_3 and $\bar{x}$ in that respective order.

4. Estimation of the Standard Deviation

The same sampling experiment was used to evaluate properties of different estimators of the standard deviation, σ. Two estimators were considered,

$$\tilde{\sigma} = 0.591\omega = 0.591(x_{(3)} - x_{(1)})$$

$$\tilde{\tilde{\sigma}} = 2.205y_1 = 2.205(x'' - x').$$

The estimate based on the range, ω, is the usual estimate for very small sample sizes, but again, if contamination is feared, one might want to use $\tilde{\tilde{\sigma}}$, the estimate based on the range of the closest two. The factors, 0.591 and 2.205, make the estimates unbiased in the null case. Lieblein [1955] has shown that $\tilde{\tilde{\sigma}}$ is quite inefficient compared to $\tilde{\sigma}$ in the null case, in fact

$$\{E(\tilde{\sigma} - \sigma)^2\}^{1/2} = 0.524\sigma$$

$$\{E(\tilde{\tilde{\sigma}} - \sigma)^2\}^{1/2} = 0.826\sigma.$$

Here, just as for the mean, the range of just two true duplicates provides a better estimate than $\tilde{\tilde{\sigma}}$.

The bias and the root mean square error of $\tilde{\sigma}$ and $\tilde{\tilde{\sigma}}$ as determined from the sampling experiment are graphed in units of σ in figure 4. These graphs are for the model in which there is exactly one contaminant in the sample. Graphs for the 100γ percent contamination model (corresponding to figures 2 and 3 for the mean) are not included in this note, but they also indicate the superiority of $\tilde{\sigma}$ over $\tilde{\tilde{\sigma}}$ when all contaminants come from the same source and $\delta \leq 3$.

5. References

Anscombe, F. J., Rejection of outliers, Technometrics **2,** 123–147 (1960).

Dixon, W. J., Rejection of outliers, ch.IOH in Contributions to Order Statistics (edited by A. E. Sarhan and B. G. Greenberg) (John Wiley & Sons, Inc., New York, N.Y., 1962).

Dixon, W. J. and Massey, F. J., Jr., Introduction to Statistical Analysis, pp 275–278 (McGraw-Hill Book Co., New York, N.Y., 1957).

Lieblein, Julius, Properties of certain statistics involving the closest pair in a sample of three observations, J. Res. NBS **48,** 255–268, (1955) RP2311.

Proschan, Frank, Testing suspected observations, Industrial Quality Control **13,** No. 7, 14–19, (1957).

(Paper 70B2–175)

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematics and Mathematical Physics
Vol. 70B, No. 2, April–June 1966

Realizing the Distance Matrix of a Graph

A. J. Goldman

Institute for Basic Standards, National Bureau of Standards, Washington, D.C.

(February 23, 1966)

An explicit description is given for the unique graph with as few arcs (each bearing a positive length) as possible, which has a prescribed matrix of shortest-path distances between pairs of distinct vertices. The same is done in the case when the ith diagonal matrix entry, instead of being zero, represents the length of a shortest closed path containing the ith vertex.

Key Words: Graph, distance matrix, shortest path.

Let G be a finite oriented graph with vertices $\{v_i\}_1^n$, where $n > 2$. To avoid unnecessary complications, we restrict attention to *connected* graphs, i.e., if $i \neq j$ then G contains a directed path from v_i to v_j. As additional structure, we assume associated to G a positive-valued function l_G assigning *lengths* $l_G(i, j)$ to the arcs (v_i, v_j) of G.

The *distance matrix* D_G of G has entries $d_G(i, i) = 0$ on the main diagonal; a typical off-diagonal entry $d_G(i, j)$ repersents the length of a shortest directed path in G from v_i to v_j. An arc of G is called *redundant* if its deletion leaves D_G unchanged. The graph G will be called *irreducible* if it contains no redundant arcs.

A real square matrix D with entries $d(i, j)$ is called *realizable* if there is a graph G such that $D = D_G$. Hakimi and Yau [1] showed that necessary and sufficient conditions for the realizability of D are

$$d(i, i) = 0, \tag{1}$$

$$d(i, j) > 0 \qquad \text{if } i \neq j, \tag{2}$$

$$d(i, j) \leq d(i, k) + d(k, j). \tag{3}$$

The necessity of these conditions should be clear. To prove sufficiency one need only take the arcs of G to be *all* (v_i, v_j) with $i \neq j$, and *define* l_G by $l_G(i, j) = d(i, j)$; it follows readily from (1) to (3) that $D_G = D$.

If matrix D is realizable, it clearly has a realization by an irreducible graph. Hakimi and Yau (op. cit.) showed that this irreducible representation was unique, but did not give an explicit description of it. Our first purpose in this note is to provide such a description.

THEOREM 1. *Let* G *be an irreducible representation of* D. *Arc* (v_i, v_j) *is present in* G *if and only if* $i \neq j$ *and*

$$d(i, j) < \min \{d(i, k) + d(k, j) : k \neq i, j\}. \tag{4}$$

In this case,

$$l_G(i, j) = d(i, j). \tag{5}$$

We remark that it follows that G can be constructed (simultaneously with the checking of (3)) in the following way. Replace the zeros on the main diagonal of D by ∞, obtaining a new matrix $E = (e_{ij})$. Form $E^2 = (e_{ij}^{(2)})$ using the special "matrix multiplication" often employed for shortest-path problems, i.e.,

$$e_{ij}^{(2)} = \min_k (e_{ik} + e_{kj}).$$

(D. Rosenblatt has pointed out the relation of this operation to the Peirce-Schroder relative sum; see e.g., B. Russell's "Principles of Mathematics.") In view of (3) and (4), arc (v_i, v_j) is present in G if and only if $i \neq j$ and $e_{ij} \neq e_{ij}^{(2)}$; if present, its length is given by (5).

We begin the proof by observing that G, because of its irreducibility, contains no arcs of the form (v_i, v_i). Thus arc (v_i, v_j) can be present in G only if $i \neq j$.

If arc (v_i, v_j) is present in G, it constitutes a path from v_i to v_j, and so

$$l_G(i, j) \geq d_G(i, j) = d(i, j). \tag{6}$$

If strict inequality held in (6), then there would be a shortest path P_{ij} from v_i to v_j (in G) which does not contain (v_i, v_j), and no path of G would be lengthened if each appearance of (v_i, v_j) in it were replaced by P_{ij}. Therefore (v_i, v_j) would be redundant, a contradiction. So (5) is proved.

Suppose (4) does *not* hold, i.e., there is a $k \neq i, j$ such that

$$d_G(i, j) = d(i, j) \geq d(i, k) + d(k, j) = d_G(i, k) + d_G(k, j). \tag{7}$$

Let P_{ik} be a shortest path in G from v_i to v_k, P_{kj} a shortest path from v_k to v_j, and Q_{ij} the composition of P_{ik} and P_{kj}. If arc (v_i, v_j) were present in G, then by (2), (5) and (7) it could not lie in P_{ik} or P_{kj}, and hence not in Q_{ij}. It follows from (5) and (7) that no path in

[1] S. L. Hakimi and S. S. Yau, Distance matrix of a graph and its realizability, Q. Applied Math., Jan. 1965, 305–317.

G would be lengthened if each appearance of (v_i, v_j) in it were replaced by Q_{ij}. Thus (v_i, v_j) would be redundant, a contradiction. We have proved that (4) is a necessary condition for the presence of (v_i, v_j) in G.

It only remains to rule out the possibility that (4) holds but arc (v_i, v_j) is absent from G. Let the successive vertices of a shortest path in G from v_i to v_j be $v_i, v_{k(1)}, \ldots, v_{k(m)}, v_j$ where $m \geq 1$ (because (v_i, v_j) is absent). Then by (5),

$$d(i, j) = d_G(i, j) = d(i, k(1)) + \ldots + d(k(m), j). \quad (8)$$

Repeated application of the triangle inequality (3) to the sum in (8) yields

$$d(i, j) \geq d(i, k(1)) + d(k(1), j),$$

contradicting (4). This completes the proof of the theorem.

COROLLARY. *A graph G is irreducible if and only if, for each of its arcs* (v_i, v_j),

$$l_G(i, j) = d_G(i, j) < \min \{d_G(i, k) + d_G(k, j) : k \neq i, j\}. \quad (9)$$

We pass now to a second type of "distance matrix," denoted $D_G^* = (d^*(i, j))$, obtained from D by changing the main diagonal's entries from $d_G(i, i) = 0$ to $d_G^*(i, i)$, the length of a shortest *closed* path of G which contains v_i.

THEOREM 2. *A matrix* D^* *is realizable as a* D_G^* *if and only if its entries* $d^*(i, j)$ *satisfy*

$$d^*(i, j) > 0, \quad (10)$$

$$d^*(i, j) \leq d^*(i, k) + d^*(k, j), \quad (11)$$

$$d^*(i, i) \leq \min \{d^*(i, j) + d^*(j, i) : j \neq i\}. \quad (12)$$

The necessity of (10) and (11) should be clear. As for (12), observe that any closed path C of G containing v_i and at least one other vertex can be regarded as consisting of a path from v_i to some other vertex v_j of C, followed by a path from v_j back to v_i; the minimum possible lengths of these two paths are $d_G^*(i, j)$ and $d_G^*(j, i)$, respectively. Thus the shortest closed path containing v_i and v_j $(j \neq i)$ has length $d_G^*(i, j) + d_G^*(j, i)$, and so

$$d_G^*(i, i) \leq \min \{d_G^*(i, j) + d_G^*(j, i) : j \neq i\}, \quad (13)$$

from which the necessity of (12) follows. Note that equality holds in (13) unless $(v_i, v_i) \in G$. (If our definition of "graph" were restricted to exclude arcs of the form (v_i, v_i), then equality would hold in (12).)

The sufficiency proof is as for D_G, except that the realizing graph is given an arc (v_i, v_i) for each index i such that strict inequality holds in (12).

We now assume the definitions of "redundant" and "irreducible" modified to apply to D_G^* rather than D_G. The analog of theorem 1 requires no new arguments. The conclusion is that if D^* can be realized as a D_G^*, it has a unique irreducible realization, whose graph G is found as follows. Change the main diagonal terms of D^* to zero, obtaining a matrix D satisfying (1) to (3). We have previously described how to construct the unique irreducible graph H such that $D_H = D$. Adjoin to H an arc (v_i, v_i) for each i such that strict inequality holds in (12), and let the length of this arc be $d^*(i, i)$.

(Paper 70B2–176)

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematics and Mathematical Physics
Vol. 70B, No. 2, April–June 1966

Pairs of Nonsingular Matrices[1]

Karl Goldberg

Institute for Basic Standards, National Bureau of Standards, Washington, D.C.

(February 16, 1966)

Let R_1 and R_2 be m by n matrices of rank m. Let S_1 and S_2 be n-m by n matrices of rank n-m such that $R_1S_1^T = R_2S_2^T = 0$. Then $R_1R_2^T$ is nonsingular if and only if $S_1S_2^T$ is nonsingular, in which case $R_2^T(R_1R_2^T)^{-1}R_1 + \{S_2^T(S_1S_2^T)^{-1}S_1\}^T$ equals the identity matrix of order n.

Key Words: Matrices (pairs of nonsingular).

Let $\mathcal{R}_{mn}$ denote the set of m by n matrices of rank m, with entries from a field of characteristic 0. Given $R \in \mathcal{R}_{mn}$ let $\mathcal{N}(R)$ denote the set of $S \in \mathcal{R}_{n-m,\,n}$ such that $RS^T = 0$. Note that $S \in \mathcal{N}(R)$ if and only if $R \in \mathcal{N}(S)$.

We assume as known the following results for $R \in \mathcal{R}_{mn}$ and $S \in \mathcal{N}(R)$:

LEMMA 1. $XR = 0$ if and only if $X = 0$.

LEMMA 2. $RY^T = 0$ if and only if $Y = ZS$, for some matrix Z.

The obvious stipulations are that X, Y, and Z have m,n and n-m columns respectively, and Y and Z have the same number of rows. Using these lemmas we prove:

THEOREM. *If* $R_1, R_2 \in \mathcal{R}_{mn}$, $S_1 \in \mathcal{N}(R_1)$, $S_2 \in \mathcal{N}(R_2)$ *then* $R_1R_2^T$ *is nonsingular if and only if* $S_1S_2^T$ *is nonsingular, in which case*

$$R_2^T(R_1R_2^T)^{-1}R_1 + \{S_2^T(S_1S_2^T)^{-1}S_1\}^T = I_n,$$

where I_n *is the identity matrix of order* n.

Suppose $R_1R_2^T$ is singular. Then there exists an $X \neq 0$ such that $XR_1R_2^T = 0$.

Let $Y = XR_1$. By Lemma 1, $Y \neq 0$. We have $R_2Y^T = R_2R_1^TX^T = (XR_1R_2^T)^T = 0$.

By Lemma 2, this implies that there exists a Z such that $Y = ZS_2$. Clearly $Z \neq 0$. We have $(S_1S_2^T)Z^T = S_1Y^T = S_1R_1^TX^T = 0$ (because $S_1R_1^T = (R_1S_1^T)^T = 0$), from which we conclude that $S_1S_2^T$ is singular.

The converse is proved in the same way, interchanging R_1 and S_1, R_2 and S_2. Thus $R_1R_2^T$ is singular if and only if $S_1S_2^T$ is singular.

Now suppose $R_1R_2^T$ and $S_1S_2^T$ are nonsingular. Let

$$M = R_2^T(R_1R_2^T)^{-1}R_1 + \{S_2^T(S_1S_2^T)^{-1}S_1\}^T - I_n$$

$$= R_2^T(R_1R_2^T)^{-1}R_1 + S_1^T(S_2S_1^T)^{-1}S_2 - I_n.$$

We wish to prove that $M = 0$. We have

$$R_1M = R_1R_2^T(R_1R_2^T)^{-1}R_1 + R_1S_1^T(S_2S_1^T)^{-1}S_2 - R_1$$

$$= R_1 + 0 - R_1$$

$$= 0.$$

Similarly $S_2M = 0$.

By Lemma 2, $R_1M = 0$ implies that there exists an N such that $M^T = NS_1$. Then

$$0 = (S_2M)^T = M^TS_2^T = NS_1S_2^T.$$

Since $S_1S_2^T$ is nonsingular, we conclude that $N = 0$, whence $M = 0$. This proves the theorem.

The following example shows that the characteristic roots (other than 0) of $R_1R_2^T$ and $S_1S_2^T$ need not have any relationship. Let

$$R_i = A_i(I_m\ 0_{m,\,n-m}) \qquad i = 1,2$$

$$S_i = B_i(0_{n-m,\,m}\ I_{n-m})$$

where A_1, A_2 and B_1, B_2 are *any* nonsingular matrices of orders m and $n-m$ respectively. Then $R_1, R_2 \in \mathcal{R}_{mn}$, $S_1 \in \mathcal{N}(R_1)$, $S_2 \in \mathcal{N}(R_2)$, but $R_1R_2^T = A_1A_2^T$ and $S_1S_2^T = B_1B_2^T$. These latter two matrices are related only in the fact that both are nonsingular.

This is in direct contrast to the known result that a characteristic root of FG (F *and* G^T matrices of the same dimensions) is a characteristic root of GF, with the possible exception of a characteristic root equal to 0; i.e., FG may be singular and GF may be nonsingular, or vice-versa.

[1] This work arose from some matrix-theoretic questions posed by Dr. U. Fano.

Yet this result can be translated into one similar to our theorem. Since 1 is either a characteristic root of both FG and GF or neither, it follows that $I-FG$ is nonsingular if and only if $I-GF$ is nonsingular. If both are nonsingular it is easy to show that

$$(I-FG)^{-1}-F(I-GF)^{-1}G=I_p,$$

where p is the number of rows of F (and columns of G).

Finally we note that if R_1, R_2, S_1, S_2 are as in the theorem and A is nonsingular matrix of order n, then

$$B=R_1AR_2^T,\ C=S_2A^{-1}S_1^T$$

are nonsingular together in which case

$$R_2^TB^{-1}R_1A+A^{-1}S_1^TC^{-1}S_2=I_n.$$

This follows from the fact that $R_1A\epsilon\mathscr{R}_{mn}$ and $S_1(A^T)^{-1}\epsilon\mathscr{N}(R_1A)$.

(Paper 70B2–177)

JOURNAL OF RESEARCH of the National Bureau of Standards – B. Mathematics and Mathematical Physics
Vol. 70B, No. 2, April–June 1966

Upper Bounds for the Determinant of a Row Stochastic Matrix

Karl Goldberg

Institute for Basic Standards, National Bureau of Standards, Washington, D.C.

(February 16, 1966)

If $A=(a_{ij})$ is a row stochastic matrix of order n then $|\det A| \leq (1-\sum_{j=1}^{n} \min_i a_{ij})^{n-1}$. If α is a 1 by n real vector such that every element of αA is nonnegative then $|\det A| \leq s(\alpha)/|g(\alpha)|$, where $s(\alpha)$ is the sum of the elements of α and $g(\alpha)$ is the element of α of greatest absolute value. The conditions for equality are determined in both cases.

Key Words: Determinants, matrices (row stochastic), upper bounds.

It is known that *if* A *is a row stochastic matrix then* $|\det A| \leq 1$ *with equality if and only if* A *is a permutation matrix.* We will use this result to extend itself.

The result is equivalent to the following statement about nonnegative matrices.[1] Let A be a nonnegative matrix of order n, let $r_A^{(i)}$ denote the sum of the elements in the ith row, let

$$r_A = r_A^{(1)} r_A^{(2)} \cdots r_A^{(n)}$$

and

$$R_A = \operatorname{diag}(r_A^{(1)}, r_A^{(2)}, \ldots, r_A^{(n)}).$$

Note that $r_A = 0$ if and only if some row of A is all 0's. Otherwise $R_A^{-1}A$ is row stochastic. *Thus* $|\det A| \leq r_A$ *with equality if and only if either* $r_A = 0$ *or* $A = R_A P$ *for some permutation matrix* P.

We use the following procedure. Given a row stochastic matrix A, let B be a nonsingular matrix such that $AB \geq 0$ (i.e., AB is nonnegative). Then the above result implies that

$$|\det A| \leq \frac{r_{AB}}{|\det B|}$$

with equality if and only if either $r_{AB}=0$ or $A=R_{AB}PB^{-1}$. The same procedure with $CA \geq 0$ yields a similar result. Since B (or C) need not be nonnegative we have room for improvement.

From this point on A will denote a row stochastic matrix of order n.

Lower case Greek letters will denote 1 by n real vectors including

$$\epsilon = (1\ 1\ \ldots\ 1) \text{ and } \delta_i = (0\ .\ .\ 0\ 1\ 0\ \ldots\ 0) = (\delta_{ij}).$$

For a vector α, $s(\alpha)$ will denote the sum of its elements, $g(\alpha)$ will denote its element of greatest absolute value, and $M_i(\alpha)$ will denote the matrix

$$M_i(\alpha) = \begin{bmatrix} \delta_1 \\ \cdot \\ \cdot \\ \cdot \\ \delta_{i-1} \\ \alpha \\ \delta_{i+1} \\ \cdot \\ \cdot \\ \cdot \\ \delta_n \end{bmatrix}$$

i.e., the identity matrix with the ith row replaced by α. For future clarity we note now that

$$s(\alpha) = \alpha\epsilon^T,$$

while $\epsilon^T\alpha$ is the matrix

$$\epsilon^T\alpha = \begin{bmatrix} \alpha \\ \alpha \\ \cdot \\ \cdot \\ \cdot \\ \alpha \end{bmatrix}$$

Finally $A\epsilon^T = \epsilon^T$. We shall prove:

THEOREM 1. *Let* A *be a row stochastic matrix of order* n, *and let*

$$c = \sum_{j=1}^{n} \min_i a_{ij}.$$

Then

$$|\det A| \leq (1-c)^{n-1}$$

[1] A matrix is nonnegative if each element is real and nonnegative. It is row stochastic if, in addition, each row sum equals 1.

with equality if and only if

$$A=(1-s(\beta))P+\epsilon^T\beta$$

for some vector $\beta \geq 0$ *with* $1 \geq s(\beta)$, *and some permutation matrix* P.

THEOREM 2. *Let* A *be a row stochastic matrix and* α *a real, nonzero vector such that* $\alpha A \geq 0$. *Then*

$$|\det A| \leq \frac{s(\alpha)}{|g(\alpha)|}$$

with equality if and only if either $s(\alpha)=0$, *or* α *has exactly one positive element (in the i-th position) and*

$$A=M_i(\gamma)P$$

for some permutation matrix P, *with*

$$\gamma=\frac{1}{g(\alpha)}\{(g(\alpha)+s(\alpha))\delta_i-\alpha\}.$$

To prove Theorem 1 let $c_j=\min_i a_{ij}$ and let

$$B=I-\sum_{j=1}^{n} c_j\epsilon^T\delta_j.$$

The matrix $\epsilon^T\delta_j$ has 1's in the jth column and 0's elsewhere, so that $AB=(a_{ij}-c_j)$. By the definition of the c_j, AB is nonnegative.

The row sums of AB are the elements of the vector

$$AB\epsilon^T=A\epsilon^T-\sum_{j=1}^{n} c_j\epsilon^T\delta_j\epsilon^T=(1-c)\epsilon^T.$$

Thus $r_{AB}^{(i)}=1-c$ for all i, so that

$$r_{AB}=(1-c)^n.$$

It is a simple exercise (left to the reader) to prove that

$$\det B=1-c$$

and

$$B^{-1}=I+(1-c)^{-1}\sum_{j=1}^{n} c_j\epsilon^T\delta_j \qquad c\neq 1.$$

If $c \neq 1$ then, from our previous discussion, the necessity case of Theorem 1 follows with

$$\beta=(c_1\ c_2\ .\ .\ .\ c_n).$$

In the case of sufficiency, if $A=(1-s(\beta))P+\epsilon^T\beta$ then all the row sums of A equal 1 ($A\epsilon^T=\epsilon^T$), A is nonnegative if $\beta \geq 0$, and $1 \geq s(\beta)$, $\beta=(c_1c_2\ .\ .\ .\ c_n)$ with the c_j defined as above, and $|\det A|=(1-s(\beta))^{n-1}$.

A short discussion of the value of c will complete our proof. Since A is row stochastic the sum of all of its elements is n. Thus

$$n=\sum_{j=1}^{n}\sum_{i=1}^{n} a_{ij} \geq \sum_{j=1}^{n}\sum_{i=1}^{n} c_j=nc$$

with equality ($c=1$) if and only if $a_{ij}=c_j$ for all i, j, in which case A is of rank 1. Then $\det A=1$ for $n=1$, and $\det A=0$ with $n>1$, and $A=\epsilon^T\beta$. This checks with the statement of Theorem 1 and completes our proof.

To prove Theorem 2 let $C=M_i(\alpha)$. The rows of CA are the rows of A except for the ith row which is αA. By hypothesis $\alpha A \geq 0$ so that CA is nonnegative.

The row sums of CA are 1 except for the ith row whose sum is

$$s(\alpha A)=(\alpha A)\epsilon^T=\alpha(A\epsilon^T)=\alpha\epsilon^T=s(\alpha).$$

Thus $r_{CA}=s(\alpha)$ and R_{CA} is the identity matrix transformed by replacing the 1 in the ith position on the diagonal by $s(\alpha)$. Note that, if $s(\alpha) \neq 0$, we have

$$R_{CA}^{-1}M_i(\alpha)=M_i(\alpha/s(\alpha)).$$

The determinant of C is the product of its diagonal elements. Let

$$\alpha=(a_1a_2\ .\ .\ .\ a_n).$$

Then $\det C=a_i$. By our previous discussion $|\det A| \leq r_{CA}/|\det C|$. Thus

$$|\det A| \leq \frac{s(\alpha)}{|a_i|}.$$

This inequality holds for all i; the best of the inequalities is

$$|\det A| \leq \frac{s(\alpha)}{|g(\alpha)|}.$$

Suppose $g(\alpha)=a_i$. We have equality if and only if either $s(\alpha)=0$, (whence $\alpha A=0$, $\alpha \neq 0$, so that $\det A=0$) or, if $s(\alpha) \neq 0$:

$$A=C^{-1}R_{CA}P=(R_{CA}^{-1}M_i(\alpha))^{-1}P=(M_i(\alpha/s(\alpha))^{-1}P$$

for some permutation matrix P.

But $(M_i(\alpha/s(\alpha)))^{-1}=M_i(\gamma)$ with

$$\gamma=a_i^{-1}(-a_1\ .\ .\ .\ -a_{i-1}\ s(\alpha)\ -a_{i+1}\ .\ .\ .\ -a_n).$$

Since $A=M_i(\gamma)P$ is nonnegative we must have $a_j \leq 0$ for $j \neq i$. This completes the proof of Theorem 2.

(Paper 70B2–178)

JOURNAL OF RESEARCH of the National Bureau of Standards—B. Mathematics and Mathematical Physics
Vol. 70B, No. 2, April–June 1966

Groups Preserving Ordering in Vectors

Karl Goldberg

Institute for Basic Standards, National Bureau of Standards, Washington, D.C.

(February 16, 1966)

The group of all nonsingular matrices taking the set of ordered 1 by n real vectors onto itself is determined. It is shown to be homomorphic to the symmetric group on $n-1$ letters. A similar result is found for the subset of nonnegative vectors: its group is homomorphic to the symmetric group on n letters.

Key Words: Vectors (ordered, nonnegative), matrices (groups of).

Throughout this note (unless otherwise stated) all vectors are 1 by n, all matrices are n by n, and all have real entries. Lower case Greek letters will denote vectors.

A vector $\alpha=(a_1a_2\ .\ .\ .\ a_n)$ will be called *ordered* if

$$a_1 \geqslant a_2 \geqslant .\ .\ . \geqslant a_n.$$

Let V denote the set of all ordered vectors, and V_0 the subset of nonnegative ones. Our purpose is to describe the groups of nonsingular matrices which take V onto V, and V_0 onto V_0, respectively.

We will need the following definition:

$$P_\pi(\tau)=\sum_{i=1}^{n} t_i E_{i,\,\pi(i)}$$

where π is an element of the symmetric group $\mathcal{S}_n$ (i.e., π is a permutation of 1,2, . . ., n), $\tau=(t_1t_2\ .\ .\ .\ t_n)$, and $E_{i,j}$ is the elementary matrix with 1 in the i, j position and 0 elsewhere. In other words, $P_\pi(\tau)$ is the permutation matrix corresponding to π with the 1 in the ith row replaced by t_i for each $1=1,2,\ .\ .\ .,\ n$. Our results are

THEOREM 1. *Let* $\mathrm{M(V)}$ *denote the group of all nonsingular matrices* M *such that* $\mathrm{VM=V}$ *(with a similar definition for* $\mathrm{M(V_0)}$*). Then*

$$\mathrm{M(V)}=\{\mathrm{K^{-1}P_\pi(\tau)K}+\gamma^{T}\epsilon:\pi\epsilon\mathcal{S}_n,\ \pi(\mathrm{n})=\mathrm{n};\ \tau>0;\ \epsilon\gamma^{T}\neq-\mathrm{t_n}\}$$

$$\mathrm{M(V_0)}=\{\mathrm{K^{-1}P_\pi(\tau)K}:\pi\epsilon\mathcal{S}_n;\ \tau>0\}$$

where K *is the matrix with ones on and below the main diagonal and zeros elsewhere,* $\tau=(\mathrm{t_1t_2\ .\ .\ .\ t_n})$, *and* $\epsilon=(1\ 1\ .\ .\ .\ 1)$.

THEOREM 2. *Let* $\mathrm{D}(\tau)=\mathrm{diag}\ (\mathrm{t_1t_2\ .\ .\ .\ t_n})$ *for* $\tau=(\mathrm{t_1t_2\ .\ .\ .\ t_n})$. *Define:*

$$\mathrm{N}=\{\mathrm{K^{-1}D}(\tau)\mathrm{K}+\gamma^{\mathrm{T}}\epsilon:\tau>0;\ \epsilon\gamma^{\mathrm{T}}\neq-\mathrm{t_n}\}$$

$$\mathrm{N_0}=\{\mathrm{K^{-1}D}(\tau)\mathrm{K}:\tau>0\}.$$

Then $\mathrm{M(V)/N}\cong\mathcal{S}_{n-1}$ *and* $\mathrm{M(V_0)/N_0}\cong\mathcal{S}_n$.

We begin with a proof of the results for V_0. We note that

$$K^{-1}=\begin{bmatrix} 1 & & & \\ -1 & 1 & 0 & \\ & -1 & 1. & \\ & & .\ & .\ \\ & & 0\ & .-1\ 1 \end{bmatrix}$$

so that

$$\alpha K^{-1}=(a_1-a_2\ a_2-a_3\ .\ .\ .\ a_{n-1}-a_n\ a_n). \qquad (1)$$

It follows that $\alpha\epsilon V_0$ if and only if $\alpha K^{-1}\geqslant 0$.

Let S denote the set of all nonnegative vectors. We have shown that

$$V_0K^{-1}=S.$$

Thus

$$V_0M=V_0 \text{ iff } S(KMK^{-1})=S.$$

In other words:

$$M(V_0)=K^{-1}M(S)K \qquad (2)$$

and our problem is reduced to describing $M(S)$.

By considering those vectors with exactly one 1 and otherwise zero entries, it is easy to see that any matrix which takes all nonnegative vectors into nonnegative vectors is itself nonnegative. To be a member of $M(S)$ both the matrix and its inverse must have that property. But a matrix and its inverse are both nonnegative if and only if it has exactly one positive entry in each row and column, i.e., if it is of the form $P_\pi(\tau)$ with $\tau>0$. Thus

$$M(S)=\{P_\pi(\tau):\pi\epsilon\mathcal{S}_n;\ \tau>0\}.$$

211-570 O-66—3

Together with (2), this proves our description of $M(V_0)$ in Theorem 1.

Now let f denote the mapping of $M(V_0)$ onto $\mathcal{S}_n$ defined by

$$f(K^{-1}P_\pi(\tau)K)=\pi^{-1}.$$

This is a homomorphism because

$$P_{\pi_1}(\tau)P_{\pi_2}(\sigma)=P_{\pi_2\pi_1}(\rho)$$

with $r_i=t_is_{\pi_1(i)}$ for $i=1, 2, \ldots, n$ (where $\tau=(t_i)$, $\sigma=(s_i)$, $\rho=(r_i)$). The kernel of f is the set of elements $K^{-1}P_e(\tau)K$ which are taken into the identity permutation e. But $P_e(\tau)=D(\tau)$ so that the kernel of f is N_0. By the first law of homomorphism we conclude that the factor group $M(V_0)/N_0$ is isomorphic to $\mathcal{S}_n$.

The case for V is slightly different. From (1) we see that $\alpha\epsilon V$ if and only if the first $n-1$ entries of αK^{-1} are nonnegative. Let S^* be the set of such vectors. As before we get

$$M(V)=K^{-1}M(S^*)K. \tag{3}$$

By considering the vectors $(0\ 0\ \ldots\ 0\pm1)$ and those with exactly one 1 in the first $n-1$ positions and zeros elsewhere, we see that a matrix taking all elements of S^* into elements of S^* must have the form

$$A=\left(\begin{array}{c|c} A_0 & \beta_0^T \\ \hline 0 & d \end{array}\right)$$

where A_0 is a nonnegative matrix of order $n-1$.

For A to be a member of $M(S^*)$ its inverse must be of the same form. We have

$$A^{-1}=\left(\begin{array}{c|c} A_0^{-1} & \gamma_0^T \\ \hline 0 & d^{-1} \end{array}\right), \qquad \gamma_0^T=-d^{-1}A_0^{-1}\beta_0^T$$

and thus A_0^{-1} is required to be nonnegative. As before, we conclude from the fact that both A_0 and A_0^{-1} are nonnegative that

$$A_0=P_{\pi_0}(\tau_0) \qquad \pi_0\epsilon\mathcal{S}_{n-1},\ \tau_0>0$$

(with τ_0 a 1 by $n-1$ vector).

Let $\pi\epsilon\mathcal{S}_n$ be such that $\pi(i)=\pi_0(i)$ for $i=1, 2, \ldots, n-1$ and $\pi(n)=n$. Then we can write A as

$$A=P_\pi(\tau)+\beta^T\epsilon_0 \qquad \pi\epsilon\mathcal{S}_n,\ \tau=(\tau_0, t_n)>0 \tag{4}$$

with $\beta=(b_1b_2\ \ldots\ b_n)$ and $\epsilon_0=(0\ 0\ \ldots\ 0\ 1)$; i.e.,

$$\beta^T\epsilon_0=\begin{pmatrix} 0 & \beta^T \end{pmatrix}.$$

The only further restriction is that the element d in the lower right-hand corner be nonzero so that A will be nonsingular. Clearly

$$d=t_n+b_n$$

so we require that $b_n\neq -t_n$. Since $b_n=\epsilon_0\beta^T$ this can be written

$$\epsilon_0\beta^T\neq -t_n. \tag{5}$$

Now we return to (3) and conclude that the elements of $M(V)$ are exactly those of the form $K^{-1}AK$ restricted by (5). We note that

$$\epsilon_0K=\epsilon.$$

Let

$$\gamma^T=K^{-1}\beta^T$$

whence

$$\epsilon_0\beta^T=\epsilon_0K\gamma^T=\epsilon\gamma^T$$

and our restriction for nonsingularity becomes

$$\epsilon\gamma^T\neq -t_n.$$

This completes the proof of Theorem 1.

Now let f' be the mapping of $M(V)$ onto $\mathcal{S}_{n-1}$ defined by

$$f'(K^{-1}P_\pi(\tau)K+\gamma^T\epsilon)=\{\lambda(\pi)\}^{-1}$$

where $\lambda(\pi)(i)=\pi(i)$ for $i=1, 2, \ldots, n-1$. This is well-defined, and is a homomorphism because $\lambda(\pi_2\pi_1)=\lambda(\pi_2)\lambda(\pi_1)$ when $\pi_1(n)=\pi_2(n)=n$,

$$(K^{-1}P_{\pi_1}(\tau)K+\gamma_1^T\epsilon)(K^{-1}P_{\pi_2}(\sigma)K+\gamma_2^T\epsilon)$$

$$=K^{-1}P_{\pi_2\pi}(\rho)K+\gamma^T\epsilon$$

(with ρ as before), and

$$\gamma^T=K^{-1}P_{\pi_1}(\tau)K\gamma_2^T+\{\epsilon\gamma_2^T+\epsilon K^{-1}\sigma^T\}\gamma_1^T.$$

(Note that $\epsilon\gamma^T-r_n=(\epsilon\gamma_1^T-t_n)(\epsilon\gamma_2^T-s_n)$.)

As before it is easy to show that the kernel of f' is N whence $M(V)/N\cong\mathcal{S}_{n-1}$, and Theorem 2 is proved.

The method of proof shows that similar results hold for

$$M(SL)=L^{-1}M(S)L,\ M(S^*L)=L^{-1}M(S^*)L$$

with L any nonsingular matrix. Likewise, the results for S^* can be extended to the set of vectors whose first k entries are nonnegative.

(Paper 70B–179)

JOURNAL OF RESEARCH of the National Bureau of Standards – B. Mathematics and Mathematical Physics
Vol. 70B, No. 2, April–June 1966

Publications of the National Bureau of Standards*

Selected Abstracts

The solution to a nonlinear Lamm equation in the Faxén approximation, I. H. Billick and G. H. Weiss, *J. Res. NBS* **70A,** *No. 1 (Jan.–Feb. 1966), 75 cents.*
An exact solution in the Faxén approximation is given for the Lamm equation in which the sedimentation coefficient is related to concentration as $s = s_0(1 - kc)$. It is shown that the solution in this case can be expressed in terms of the solution to the linear case ($k = 0$) with a modified argument. The boundary sharpening phenomenon expresses itself very clearly in the solution presented here.

A bounded automorphic form of dimension zero is constant, M. I. Knopp, J. Lehner, and M. Newman, *Duke Math. J.* **32,** *No. 3, 457–460 (Sept. 1965).*
It is proved that a bounded automorphic form of dimension zero is constant. It is shown that this implies the known result that an abelian integral of the first kind on a compact Riemann surface cannot have all real periods. Finally, a simple proof is given of the result that a bounded automorphic function is constant.

Density distribution of polymer segments in the vicinity of an absorbing interface, C. A. J. Hoeve, *J. Chem. Phys.* **43,** *No. 9, 3000–3008 (Nov. 1, 1965).*
At a small distance from the interface corresponding to the effective thickness of the segments, the density drops suddenly by an amount that is the greater, the stiffer the chain. Beyond this distance the density is exponential in the distance from the interface for long chains and relatively weak adsorption.

Elastic stress-strain relations in perfect elastic fluids, B. Bernstein, E. Kearsley, and L. Zapas, *Trans. Soc. Rheol.* **9,** *Pt. 1, 27–39 (1965).*
The theory of perfect elastic fluids deals with the non-equilibrium thermodynamics of finite viscoelastic deformation. The thermodynamics of finite elastic strain and of perfect elastic fluids are discussed. It is shown that the stress-strain relations for perfect elastic fluids may be written in a way which appears formally identical to those in elasticity theory, but the form of this dependence depends on past history.

Error bounds for asymptotic solutions of second-order differential equations having an irregular singularity of arbitrary rank, F. W. J. Olver and F. Stenger, *J. SIAM, Ser. B.* **2,** *No. 2, 244–249 (1965).*
Strict error bounds are established for the well-known asymptotic expansions of solutions of the differential equation

$$\frac{d^2w}{dz^2} + f(z)\frac{dw}{dz} + g(z)w = 0,$$

for large values of z, real or complex, where

$$f(z) \sim z^k \sum_{s=0}^{\infty} \frac{f_s}{z^s}, \qquad g(z) \sim z^{2k} \sum_{s=0}^{\infty} \frac{g_s}{z^s},$$

k being an arbitrary non-negative integer, and f_s, g_s constants.

Estimation of the parameters of the Hyper-Poisson distribution, E. L. Crow and G. E. Bardwell (*Proc. Symp. Classical and Contagious Discrete Distribution, Montreal, Canada, Aug. 15–20, 1963), ch. V, pp. 127–140 (Statistical Publ. Soc., Calcutta, India, 1965).*
The hyper-Poisson family of discrete distributions, a two-parameter generalization of the Poisson distributions, was introduced recently by the authors (Journal of the American Statistical Association, 59, March 1964). In this paper six different pairs of estimators (including four proposed in the previous paper) for the two parameters are presented and discussed: maximum likelihood, two moments, three moments, two moments plus zeroth frequency, mean plus first two frequencies, and two frequencies only. Three of these pairs are given by simple explicit formulas. Asymptotic variances are obtained for the three-moment estimators, and empirical variances for the three pairs of explicit estimators. Some of the estimators are applied to five examples of experimental or survey data.

Generalized functions of symmetric matrices, M. Marcus and M. Newman, *Proc. Am. Math. Soc.* **16,** *No. 4, 826–830 (Aug. 1965).*
Among other results, the following is proved: Let A be a symmetric matrix with positive entries. Then a diagonal matrix D exists having positive diagonal elements such that the matrix DAD is doubly stochastic.

Inequalities for permanents and permanental minors, R. A. Brualdi and M. Newman, *Proc. Camb. Phil. Soc.* **61,** *741–746 (Jan. 1966).*
The principal result of this paper is that for all non-negative doubly-stochastic matrices A and all α such that $0 \leq \alpha \leq 1$, $\mathrm{per}(\alpha I + (1-\alpha)A) \leq \alpha + (1-\alpha)\mathrm{per}(A)$, where $\mathrm{per}(A)$ denotes the permanent of A.

Normal subgroups of the modular group which are not congruence subgroups, M. Newman, *Proc. Am. Math. Soc.* **16,** *No. 4, 831–832 (Aug. 1965).*
A new family of normal subgroups of finite index in the modular group which are not congruence subgroups, is given.

On the asymptotic solutions of second-order differential equations having an irregular singularity of rank one, with an application to Whittaker functions, F. W. J. Olver, *J. SIAM, Ser. B.* **2,** *No. 2, 225–243 (1965).*
Strict error bounds are established for the well-known asymptotic expansions of solutions of the differential equation

$$\frac{d^2w}{dz^2} + f(z)\frac{dw}{dz} + g(z)w = 0,$$

for large values of z, real or complex, where

$$f(z) \sim \sum_{s=0}^{\infty} \frac{f_s}{z^s}, \qquad g(z) \sim \sum_{s=0}^{\infty} \frac{g_s}{z^s},$$

and f_s, g_s are constants.

Real two-dimensional representations of the modular group and related groups, J. Lehner and M. Newman, *Am. J. Math.* **87,** *No. 4, 945–954 (Oct. 1965).*
The principal result proved is the following: Put $T = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$, $R_\rho = \begin{pmatrix} 0 & -\rho \\ 1/\rho & 1 \end{pmatrix}$, $G_\rho = \{T, R_\rho\}$ where $\rho \geq 1$. Then (*i*) G_ρ is the free product of a cyclic group of order 2 and a cyclic group of order 3, (ii) G_ρ is a discrete group, (iii) every discrete faithful representation of the modular group Γ by real 2×2 matrices is conjugate to G_ρ for some $\rho \geq 1$, and (iv) G_ρ and G_σ are conjugate for $\rho, \sigma \geq 1$ if and only if $\rho = \sigma$.

The fundamental solution and Huygen's principle for decomposable differential operators, J. E. Lagnese, *Archive Rat. Mech. Anal.* **19,** *No. 4, 299–307 (Jan. 22, 1965).*
A nonparabolic linear partial differential operator L of second order is called *decomposable* if there is a coordinate system in the Riemann

space (the metric of which is defined by the coefficients of terms of second order) in which L has the form $L = \mathscr{L} + \overline{\mathscr{L}}$ and such that the same independent variable does not appear in both $\mathscr{L}$ and $\overline{\mathscr{L}}$. This paper is concerned with such operators and the principle result is an identity which relates in a rather simple manner the coefficients of the fundamental solutions (in the sense of Hadamard and Courant) of the three operators $\mathscr{L}$, $\overline{\mathscr{L}}$, and L. The form of the identity shows that if both $\mathscr{L}$ and $\overline{\mathscr{L}}$ have terminating fundamental solutions, the same must be true of L and, consequently, in the case when L is strictly hyperbolic, one may draw certain conclusions concerning the validity of Huygens' principle for L.

Similar resluts are obtained in the case when L decomposes according to $L = \sum_{k=1}^{n} \mathscr{L}_k$. Two illustrative examples are given.

Atomic lifetimes in neon I, J. Z. Klose, *Phys. Rev.* **141,** *No. 1, 181–188 (Jan. 7, 1966).*

Mean lives of a number of electronically excited atomic levels in Ne I have been determined using a method of delayed coincidence. Following a detailed description of the experimental procedure and a discussion of a series of trial runs in He I, the measured values of the mean lives of the $2p_1$ through $2p_{10}$, $3p_1$, $3p_{10}$, and $4d'_1$ (Paschen notation) levels in neutral neon are given. These lifetimes, determined from transitions with associated wavelengths extending from ≈3400 to ≈6400 Å, ranged in value from ≈14 to ≈500 nsec. The lifetimes were estimated to contain possible systematic errors varying from 5 to 20% and are presented in comparison with corresponding results of other workers.

Generalized master equation for arbitrary initial states, J. Weinstock, *Phys. Rev.* **140,** *No. 1A, A98–99 (Oct. 4, 1965).*

Exact generalized master equations, for both quantum and classical systems, are derived for completely arbitrary initial states (arbitrary initial "correlations") in the form of a density expansion. This result is a generalization of a previous equation which was restricted to initially "uncorrelated" states.

Generalized variational principles for electromagnetic junctions. Vibrations: application to the theory of waveguide, *Proc. Symp. Electromagnetic Theory and Antennas, Copenhagen, Denmark, June 1962, ed. E. C. Jordan, pp. 253–260 (Pergamon Press Inc., New York, N.Y., 1963).*

Generalized variational principles are stated for the elements—and for the associated electromagnetic fields—of the immittance matrices of waveguide junctions. The formulation applies to junctions containing arbitrary dissipative and anisotropic media, for which the underlying differential equations are not self-adjoint; and, by the use of bilinear (rather than quadratic) functional forms, permits direct treatment of off-diagonal elements of the immittance matrices.

AXLE: An axiomatic language for string transformations, K. Cohen and J. H. Wegstein, *Commun. Assoc. Compt. Mach* **8,** *No. 11, 657–661 (Nov. 1965).*

AXLE is a language designed for data manipulation. Data arranged in a linear form in a workspace is transformed according to a table of axioms, called imperatives. A transformation consists of a matching procedure, which decides where an imperative is applicable, and a replacement procedure that modifies that part of the workspace. Imperatives are applied in accordance with definitions of symbolic terms, presented systematically in an assertion table. The process of definition includes the special case of recursive assertions. Several complete programs of imperatives are given to show a few applications of the language.

Morphological classification in the National Bureau of Standards mechanical translation system, L. F. Meyer, *J. Assoc. Compt. Mach.* **12,** *No. 4, 437–472 (Oct. 1965).*

In linguistic work, morphology is the study of the rules by which words undergo changes in form. Morphological classification is the systematic organization of these rules. A detailed account of the morphological classification for Russian is given as used in the National Bureau of Standards project on the mechanical translation of Russian into English. The account includes the heuristic reasoning from which the classification system evolved, as well as complete classification tables, a description of the method of their construction, and some examples of their use.

Error bounds for asymptotic expansions of special functions in the complex plane, F. W. J. Olver, *Proc. Symp. on Error in Digital Computation, U. S. Army Research Center, Madison, Wisconsin, April 26–28, 1965, Vol.* **2,** *pp. 55–75 (John Wiley & Sons, Inc., New York, N. Y., 1965).*

Error bounds are given for a number of different types of asymptotic expansion derived from (i) the solution of ordinary linear differential equations of the second order, (ii) infinite integrals. Similarities between the results are discussed, and applications to the special functions of mathematical physics indicated.

Much of the paper is in the nature of a survey, but new results are given for asymptotic solutions, with respect to a parameter, in a region containing a regular singularity of the differential equation, and also for the asymptotic expansion of a simple integral of Laplace type.

New approach to the theory of fluctuations in a plasma, J. Weinstock, *Phys. Rev.* **139,** *No. 2A, A388–A393 (July 19, 1965).*

A rigorous but simple method is presented for calculating autocorrelation functions (fluctuations) of nonequilibrium plasmas—including inhomogeneous and nonstationary plasmas—in external fields. This method is based upon the derivation of an exact and remarkably simple formal relation between autocorrelation functions and the usual one-particle distribution function $f_1(\mathbf{R}, \mathbf{v}, t)$ for an explicitly defined initial value. This relation explicitly reduces the problem of calculating fluctuation spectra to the problem of solving the usual kinetic equations for $f_1(\mathbf{R}, \mathbf{v}, t)$. Consequently, the central quantity of fluctuation theory is one and the same with the central quantity of kinetic theory, and the two theories are completely and explicitly united. To first order in the plasma parameter it is shown that one need only solve the linearized Vlasov equation for $f_1(\mathbf{R}, \mathbf{v}, t)$, and when this solution is substituted into our formal relation we obtain a general formula for autocorrelation functions which is valid for nonstationary systems and includes the effects of the transverse motion of the plasma in addition to the longutudinal motion. For stationary systems this formula approaches the numerous calculations of previous authors in the limits where the transverse terms vanish. As a result of the transverse terms, the spectrum of scattered light can have resonant peaks at frequencies which correspond to transverse modes of oscillation as well as to the well-known longitudinal modes.

Theory of relaxation in a group of weakly coupled systems, R. L. Peterson, *Phys. Rev.* **139,** *No. 4A, A1151–A1155 (Aug. 1965).*

A general formalism for computing relaxation times characterizing two or more weakly coupled macroscopic systems is presented. The physical nature of the systems is arbitrary, although applications to spin systems are briefly discussed. The main assumptions are that each system is internally in equilibrium with a well-defined temperature, that the systems are weakly coupled to one another, and that the Hamiltonians of the systems form a commuting set. No high-temperature approximations are used. The formalism is presented in an effort to unify in part the approaches which have been developed for many special physical situations, and to show the form some relaxation times take when the high-temperature approximations are not used. It is shown that when one of two coupled systems is a "Zeeman" system, the (spin) relaxation time is proportional to the magnetic adiabatic susceptibility.

On radiation of electromagnetic and electroacoustic waves in a plasma, J. R. Wait, *Appl. Sci. Res.* **11,** *Sec. B., 423–432 (June 11, 1965).*

Radiation from current distributions in lossless compressible plasma media is considered. A linearized theory is used such that the isotropic electron plasma is regarded as a single fluid continuum. It is found that a considerable portion of the power is radiated as an electroacoustic-type wave. Some specialized results of other investigators are recovered.

Other NBS Publications

J. Res. NBS 70A, (Phys. and Chem.), No. 1, (Jan.–Feb. 1966), $1.00.

Optical and magnetic spectra of bis-*N*-propylsalicylaldiminato copper (II). C. W. Reimann, G. F. Kokoszka, and H. C. Allen, Jr.

Phase equilibria in the system niobium pentoxide—germanium dioxide. E. M. Levin.

Phase equilibria in the system niobium pentoxide-boric oxide. E. M. Levin.

The solution to a nonlinear Lamm equation in the Faxén approximation. I. H. Billick and G. H. Weiss. (See above abstracts.)

A line formula notation system for coordination compounds: III Deviations from idealized configurations. E. Silverton and R. F. Pasternack.

The spherulitic crystallization of isotactic polypropylene from solution: On the evolution of monoclinic spherulites from dendritic chain-folded crystal precursors. F. Khoury.

Wavelengths, intensities, and Zeeman patterns in ytterbium spectra (Yb I, II, III, IV). W. F. Meggers and C. H. Corliss.

J. Res. NBS 70A (Phys. and Chem.), No. 2 (Mar.–Apr. 1966), $1.00.

Mechanism of the depolymerization of polytetrafluoroethylene with pyrolytic and radiolytic initiation. Roland E. Florin, M. S. Parker, and L. A. Wall.

Effect of some halogenated hydrocarbons on the flame speed of methane. C. Halpern.

Rupture-disk ampoule for anhydrous addition of hydrogen fluoride. A. R. Glasgow, Jr.

Further studies in the annealing of a borosilicate glass. S. Spinner and A. Napolitano.

Infrared spectra of the hydrated borates. C. E. Weir.

Interpretation of the solution absorption spectra of the $(PuO_2)^{++}$ and $(NpO_2)^{+}$ ions. J. C. Eisenstein and M. H. L. Pryce.

Vapor pressure and heat of sublimation of rhenium. E. R. Plante and R. Szwarc.

Steady-state response of silicon radiation detectors of the diffused *p-n* junction type to x rays. II: Photodiode mode of operation. K. Scharf and J. H. Sparrow.

Absolute isotopic abundance ratios and the atomic weight of a reference sample of chromium. W. R. Shields, T. J. Murphy, E. J. Catanzaro, and E. L. Garner.

J. Res. NBS 70C (Engr. and Instr.), No. 1 (Jan.–Mar. 1966), 75 cents.

Coulometric calibration of microvolumetric apparatus. G. Marinenko and J. K. Taylor.

Effect of temperature and notch geometry on the tensile behavior of a titanium alloy. W. D. Jenkins and W. A. Willard.

Measurement standards for low and medium peak pulse voltages. A. R. Ondrejka and P. A. Hudson.

Temperature coefficient of rf permeability measurement using an impedance bridge as an equality indicating device. A. L. Rasmussen.

A test apparatus for the study of forced air-mixing devices. T. K. Faison, J. C. Davis, and P. R. Achenbach.

A table of radiation characteristics for uniformly spaced optimum endfire arrays with equal sidelobes, M. T. Ma and D. C. Hyovalti, NBS Mono. 95, (Dec. 10, 1965), 45 cents.

Safety rules for the installation and maintenance of electric supply and communication lines, Supplement 1 to NBS Handbook 81 (Dec. 15, 1965).

Calibration and test services of the National Bureau of Standards, NBS Misc. Publ. 250, 1965 edition (Oct. 28, 1965). $1.00. Supersedes 1963 edition.

Standard Reference Materials: Methods for the chemical analysis of NBS copper-base spectrochemical standards, R. K. Bell, NBS Misc. Publ. 260–7 (Oct. 25, 1965), 60 cents

Standard Reference Materials: Analysis of uranium concentrates at the National Bureau of Standards, M. S. Richmond, NBS Misc. Publ. 260–8, (Dec. 1, 1965), 55 cents.

Standard Reference Materials: Half lives of materials used in the preparation of standard reference materials of nineteen radioactive nuclides issued by the National Bureau of Standards, S. C. Anspach, L. M. Cavallo, S. B. Garfinkel, J. M. R. Hutchinson, and C. N. Smith, NBS Misc. Publ. 260–9 (Nov. 15, 1965), 15 cents.

Standard Reference Materials: Homogeneity characterization of NBS spectrometric standard II: Cartridge brass and low-alloy steel, H. Yakowitz, D. L. Vieth, K. F. J. Heinrich, and R. E. Michaelis, NBS Misc. Publ. 260–10, (Dec. 14, 1965), 30 cents.

Automotive lifts, CS142–65 (Sept. 1, 1965), 10 cents. Supersedes CS142–62.

Acrylonitrile-butadiene-styrene (ABS) plastic drain, waste, and vent pipe and fittings, CS270–65 (Apr. 1, 1965). 15 cents.

Polyvinyl chloride (PVC) plastic drain, waste, and vent pipe and fittings, CS272–65 (Apr. 1, 1965). 15 cents.

Standard stock sizes of machined tool steel bars (flast and squares), SPR267–65 (Aug. 15, 1965). 10 cents.

Accuracy in electrical and radio measurements and calibrations, 1965, ed. R. C. Powell, NBS Tech. Note 262–A (June 15, 1965), 50 cents.

Voltage ratio detector for millivolt signals, J. R. Houghton, NBS Tech. Note 266 (Dec. 13, 1965), 15 cents.

Organic chemistry: Radioactive carbohydrates, sugars in solution, aldol condensations, molecular structure, synthesis of selected compounds, air pollution studies, reference materials (organic), July 1964 to June 1965, ed. H. S. Isbell, NBS Tech. Note 274 (Dec. 3, 1965), 60 cents.

Radiochemical analysis: Activation analysis, instrumentation, radiation techniques, and radioisotope techniques, July 1964 to June 1965, ed. J. R. DeVoe, NBS Tech. Note 276 (Jan. 7, 1966), $1.00.

Flux averaging devices for the infrared, S. T. Dunn, NBS Tech. Note 279 (Dec. 9, 1965), 30 cents.

A peak ac-dc voltage comparator for use in a standards laboratory, L. A. Marzetta, NBS Tech. Note 280 (Jan. 17, 1966), 25 cents.

Materials for PLACEBO V, W. C. Watt, NBS Tech. Note 281 (Jan. 17, 1966), 50 cents.

Keypunch controls for string-punching of statistical data, M. J. Brennan, NBS Tech. Note 282 (Feb. 11, 1966), 25 cents.

A method for obtaining the parameters of electron-density profiles from topside ionograms, R. S. Lawrence and M. Hallenbeck, NBS Tech. Note 315 (Aug. 3, 1965), 25 cents.

Numerical simulation of ionospheric wave interaction experiments, T. M. Georges, NBS Tech. Note 325 (Oct. 25, 1965), 30 cents.

Adhesive bonding of various materials to hard tooth tissues. II. Bonding to dentin promoted by a surface-active comonomer, R. L. Bowen, J. Dental Res. **44,** No. 5, 895–902 (Sept.–Oct. 1965).

Adhesive bonding of various materials to hard tooth tissues. III. Bonding to dentin improved by pretreatment and the use of surface-active comonomer, R. L. Bowen, J. Dental Res. **44,** No. 5, 903–905 (Sept.–Oct. 1965).

Adhesive bonding of various materials to hard tooth tissues. IV. Bonding to dentin, enamel, and fluorapatite improved by the use of a surface-active comonomer, R. L. Bowen, J. Dental Res. **44,** No. 5, 906–911 (Sept.–Oct. 1965).

Approach to simple exponential decay in vibrational relaxation, T. Carrington, J. Chem. Phys. **43,** No. 2, 473–479 (July 15, 1965).

Experimental atomic scattering factors for magnesium oxide, G. Burley, J. Phys. Chem. Solids **26,** 1605–1613 (Apr. 8, 1965).

Major revisions made in new dry cell standard W. J. Hamer, Mag. Std. **36,** No. 10, 306–308 (Oct. 1965).

Phase equilibria in the system aluminum oxide-tungsten oxide, J. L. Waring, J. Am. Ceram. Soc. **48,** No. 9, 493–494 (Sept. 1965).

Relative signs of nuclear spin couplings in $^1H^{11}B^{19}F_2$, E. B. Whipple, T. H. Brown, T. C. Farrar, and T. D. Coyle, J. Chem. Phys. **43,** No. 5, 1841–1842 (Sept. 1, 1965).

The crystal structure of barium tetraborate, $BaO{\cdot}2B_2O_3$, S. Block and A. Perloff, Acta Cryst. **19,** Pt. 3, 297–300 (Sept. 1965).

The system WO_3–B_2O_3, E. M. Levin, J. Am. Ceram. Soc. **48,** No. 9, 491–492 (Sept. 1965).

Vibrational fundamentals of CF_2N_2 from the ultraviolet absorption spectrum, J. D. Simmons, I. R. Bartky, and A. M. Bass, J. Mol. Spectr. **17,** No. 1, 48–49 (July 1965).

A precision noise-comparator, M. G. Arthur, C. M. Allred, and M. K. Cannon, IEEE Trans. Instr. Meas. **IM–13,** No. 4, 301–305 (Dec. 1964).

A variable characteristic impedance coaxial line, J. E. Cruz and R. L. Brooke, IEEE Trans. Micro. Theory Tech. **MTT–13,** No. 4, 477–478 (July 1965).

Impact of new technology on the forest industries, R. W. Smith, Jr., Proc. 2d Annual Forest Industries Marketing Conference, June 16–17, 1965, pp. 119–130 (University of Oregon Press, Eugene, Oregon, June 16, 1965).

Study of methods for estimating loudness, E. L. R. Corliss and G. E. Winzer, J. Acoust. Soc. Am. **38,** No. 3, 424–428 (Sept. 1965).

Acoustical thermometer, H. H. Plumb and G. Cataland, Science **150,** No. 3693, 155–161 (Oct. 8, 1965).

An international comparision of inductive voltage divider calibrations at 400 to 1000° Hz, W. C. Sze, A. F. Dunn, and T. L. Zapf, IEEE Trans. Instr. Meas. **IM-14,** No. 3, 124–131 (Sept. 1965).

Precise voltage-ratio measurement, T. L. Zapf, Electro-Technol. **76,** No. 4, 95–102 (Oct. 1965).

An image source technique for calculating reflection of gamma rays or neutrons, C. Eisenhauer, Health Phys. **11,** 1145–1154 (1965).

Angular scattering law for the moon at 6-meter wavelength, W. K. Klemperer, J. Geophys. Res. Letters **70,** No. 15, 3798–3800 (Aug. 1, 1965).

Dissociation of H_2^+ by electron impact, G. H. Dunn, B. Van Zyl, and R. H. Zare, Phys. Rev. Letters **15,** No. 15, 610 (Oct. 11, 1965).

Effects of tropospheric refraction in earth-space links, K. A. Norton, Book, Progress in Radio Science 1960–1963—Radio and Troposphere, ed. F. du Castel, II, pp. 186–210 (Elsevier Publ. Co., Amsterdam, The Netherlands, 1965).

Fermi resonance in condensed CF_4 and CCl_4, S. Abramowitz and J. J. Comeford, Spectrochim. Acta **21,** 1479–1486 (1965).

Field desorption of thorium from a field-evaporated tungsten surface, R. D. Young, J. Appl. Phys. **36,** No. 9, 2656–2657 (Sept. 1965).

Laboratory measurement of the rate of the reaction $N_2 + O - NO + N$ at thermal energy, E. E. Ferguson, F. C. Fehsenfeld, P. D. Goldan, A. L. Schmeltekopf, and H. I. Schiff, Planet. Space Sci. **13,** 823–827 (1965).

Long-period very low frequency emission pulsations, W. B. Carson, J. A. Koch, J. H. Pope, and R. M. Gallet, J. Geophys. Res. **70,** No. 17, 4293–4303 (Sept. 1, 1965).

Meson and baryon resonances in relativistic SU(6), H. Harari, D. Horn, M. Kugler, H. J. Lipkin, and S. Meshkov, Phys. Rev. **140,** No. 2B, B431–B433 (Oct. 25, 1965).

Positive ion-neutral reactions in the ionosphere, E. E. Ferguson, F. C. Fehsenfeld, P. D. Goldan, and A. L. Schmeltekopf. J. Geophys. Res. **70,** No. 17, 4324–4329 (Sept. 1, 1965).

Potential-energy curves for CO and CO^+, P. H. Krupenie and S. Weissman, J. Chem. Phys. **43,** No. 5, 1529–1534 (Sept. 1, 1965).

Rotating shutter for time-resolved spectroscopy in the microsecond range, I. R. Bartky and A. M. Bass, Appl. Opt. **4,** No. 10, 1354–1356 (Oct. 1965).

Solar-flare frequency and observing-time patterns, C. S. Warwick, Astrophys. J. **142,** No. 2, 767–772 (Aug. 15, 1965).

Solution polishing of oriented single crystals, R. D. Deslattes, B. G. Simson, and A. T. Horton, Rev. Sci. Instr. **36,** No. 7, 943–944 (July 1965).

Spectrum of doubly ionized lanthanum (La III), J. Sugar and V. Kaufman, J. Opt. Soc. Am. **55,** No. 10, 1283–1285 (Oct. 1965).

Speed of sound in fluid parahydrogen, B. A. Younglove, J. Acoust. Soc. Am. **38,** No. 3, 433–438 (Sept. 1965).

Stress-strain relationships in yarns subjected to rapid impact loading. Part XI: Strain distributions resulting from rifle bullet impact, J. C. Smith, C. A. Fenstermaker, and P. J. Shouse, Textile Res. J. **35,** No. 8, 743–757 (Oct. 21, 1965).

$SU(6)_W$ photoproduction and meson-baryon scattering amplitudes, J. C. Carter, J. J. Coyne, S. Meshkov, D. Horn, M. Kugler, and H. J. Lipkin, Phys. Rev. Letters **15,** No. 8, 373–377 (Aug. 23, 1965).

An analysis of the effects of ground reflection in line-of-sight phase systems, M. C. Thompson, Jr. IEEE Trans. Ant. Prop. **AP-13,** No. 4, 564–567 (July 1965).

Conjugate observations of solar proton events: delayed ionospheric changes during twilight, H. J. A. Chivers, and J. K. Hargreaves, Planet. Space Sci. **13,** 583–592 (1965).

Cosmic-noise survey at 65 degrees (N) declination in the 5–50 Mc/s band, R. Parthasarathy and G. M. Lerfald, Monthly Notices Roy. Astron. Soc. **129,** No. 6, 395–409 (1965).

Dynamic spectral characteristics of micropulsation pearls, J. H. Pope, J. Geophys. Res. **70,** No. 15, 3595–3603 (Aug. 1, 1965).

On the determination of the electron density within discrete auroral forms in the *E* region, R. D. Hunsucker, J. Geophys. Res. **70,** No. 15, 3791–3792 (Aug. 1, 1965).

Some additional features of radar returns from the equatorial electorjet, B. B. Balsley, J. Geophys. Res. **70,** No. 13, 3175–3182 (July 1, 1965).

Chemical structures as information—representations, transformation, and calculations, S. J. Tauber, G. F. Fraction, and H. W. Hayward, Book, Colloquium on Technical Preconditions for Retrieval Center Operations, Philadelphia, Pa., Apr. 24–25, 1964, ed. B. F. Cheydleur, pp. 73–101 (Spartan Books, Inc., Washington, D. C., 1965).

Determination of hide substance in leather by the Kjeldahl method, S. Dahl, Book, The Chemistry and Technology of Leather IV, ch. 52, 45–70 (Reinhold Publ. Corp., New York, N. Y., 1965).

Determination of tellurium by cathode-ray polarography, E. J. Maienthal and J. K. Taylor, Anal. Chem. **37,** No. 12, 1516–1519 (Nov. 1965).

Digital handling of chemical structures and associated information, S. J. Tauber, Proc. 20th Natl. Conf. Association for Computing Machinery, pp. 206–216 (1965).

Electrodeposition of alloys, past, present, and future, A. Brenner, Plating **52,** No. 12, 1249–1257 (Dec. 1965).

Physical and mechanical properties of electrode-deposited copper I. Literature survey, V. A. Lamb and D. R. Valentine, Plating **52,** No. 12, 1289–1311 (Dec. 1965).

Some experience with the Hayward linear notation system, H. W. Hayward, H. M. S. Sneed, J. H. Turnipseed, and S. J. Tauber, J. Chem. Doc. **5,** No. 3, 183–189 (Aug. 1965).

The crystal and molecular structure of iodopentaborane-9, L. H. Hall, S. Block, and A. Perloff, Acta Cryst. **19,** pt. 4, 658–661 (Oct. 1965).

The use of visible and ultraviolet spectroscopy to identify carbonyl compounds in photodegraded plastics, V. E. Grady and J. R. Wright, Polymer Engr. Sci. **5,** No. 4, 284–290 (Oct. 1965).

A theoretical model for predicting thermal stratification and self pressurization of a fluid container, R. W. Arnett and D. R. Millhiser, Proc. Conf. Propellant Tank Pressurization and Stratification, Jan. 20–21, 1965, **II,** 1–16 (NASA, George C. Marshall Space Flight Center, Huntsville, Alabama, 1965).

Calibration of peak A-C to D-C comparators, D. Flach and L. A. Marzetta, (ISA 20th Annual Conference and Exhibit, Los Angeles, Calif., Oct. 4–7, 1965), ISA Preprint 14.2–3–65 (1965).

Cryogenics and space technology, R. B. Scott, Proc. XIth Intern. Congress of Refrigeration, Munich, Germany, 1963, pp. 105–114, (Pergamon Press Inc., New York, N. Y., 1965).

Evidence for an electrochemical-mechanical stress corrosion fracture in a stainless steel, H. L. Logan, M. J. McBee, and D. J. Kahan, Corrosion Sci. **5,** 729–730 (1965).

Preparation of copper crystals with low electrical resistivity, J. J. Gniewek and A. F. Clark, J. Appl. Phys. **36,** No. 10, 3358–3359 (Oct. 1965).

The world of cryogenics. III. Cryogenics at the National Bureau of Standards Boulder Laboratories, B. W. Birmingham, Cryogenics **5,** No. 3, 121–128 (June 1965).

Cesium beam atomic time and frequency standards, R. E. Beehler, R. C. Mockler, and J. M. Richardson, Metrologia **1,** No. 3, 114–131 (July 1965).

International weights and measures, C. H. Page, (ISA 20th Annual Conference and Exhibit, Los Angeles, Calif., Oct. 4–7, 1965), ISA Preprint 33.3–1–65 (1965).

Measurement standards, A. G. McNish, Intern. Sci. Tech., 58–66 (Conover-Mast. Publ., New York, N. Y., Nov. 1965).

Of time and the atom, G. E. Hudson, Phys. Today **18,** No. 8, 34–38 (Aug. 1965).

A new speculation of terrestrial helium loss, E. E. Ferguson, F. C. Fehsenfeld, and A. L. Schmeltekopf, Planet. Space Sci. **13,** 925–928 (1965).

Breadth of decay quanta in gas lasers, J. A. White, J. Opt. Soc. Am. **55,** No. 11, 1436–1442 (Nov. 1965).

Classical diagram technique for calculating thermostatic properties of Solids; application to dielectric susceptibility of paraelectrics, R. M. Wilcox, Phys. Rev. **139,** No. 4A, A1281–A1291 (Aug. 16, 1965).

Conformation of polystyrene adsorbed at the θ-temperature, R. R. Stromberg, D. J. Tutas, and E. Passaglia, J. Phys. Chem. **69,** No. 11, 3955–3963 (Nov. 1965).

Critical-point phenomena, M. S. Green, Science **150,** No. 3693, 229–236 (Oct. 8, 1965).

Density expansion of the viscosity of a moderately dense gas, J. V. Sengers, Phys. Rev. Letters **15,** No. 12, 515–517 (Sept. 20, 1965).

Differences in the characteristic electron energy-loss spectra of solid and liquid bismuth, C. J. Powell, Phys. Rev. Letters **15,** No. 22, 852–854 (Nov. 29, 1965).

Dipole moment of PCl_4F from the nonresonant microwave absorption of the vapor, A. A. Maryott and S. J. Kryder, J. Chem. Phys. **43,** No. 7, 2556–2557 (Oct. 1, 1965).

Infrared and microwave spectra of ClCN, W. J. Lafferty, D. R. Lide and R. A. Toth, J. Chem. Phys. **43,** No. 6, 2063–2070 (Sept. 15, 1965).

Investigation of the anomaly in the response of silicon semiconductor radiation detectors at low temperatures, W. R. Dodge, S. R. Domen, A. T. Hirshfeld, and D. D. Hoppes, IEEE Trans. Nuclear Sci. **NS–12,** No. 1, 295–303 (1965).

Ionization energies of the singly ionized rare earths, J. Sugar and J. Reader, J. Opt. Soc. Am. **55,** No. 10, 1286–1290 (Oct. 1965).

Microwave spectrum and barrier to internal rotation in methylsilylacetylene, W. H. Kirchhoff and D. R. Lide, Jr., J. Chem. Phys. **43,** No. 7, 2203–2213 (Oct. 1, 1965).

Modes of propagation in a bounded compressible plasma, J. R. Wait, Electronics Letters **1,** 193–194 (Sept. 1965).

Philosophical influences on radiation protection standards, L. S. Taylor, Health Phys. **11,** 859–864 (1965).

Precision refractometry of small lens-shaped objects, J. R. Meyer-Arendt, Lab. Invest. **13,** No. 5, 529–532 (1965).

Quantum statistics of fully ionized gases, W. T. Grandy and F. Mohling, Ann. Phys. **34,** No. 3, 424–464 (Oct. 1965).

Resonance in the light scattered from a plasma, J. Weinstock, Physics Letters **18,** No. 1, 21–22 (Aug. 1, 1965).

The direction of the force on a dislocation and the sign of the Burgers vector, R. DeWit, Acta Met. **13,** No. 11, 1210–1211 (1965).

Ultrasonic determination of crystalline resonances and sound velocities, using NMR techniques, R. J. Mahler, and W. H. Tanttila, J. Acoust. Soc. Am. **38,** No. 3, 429–432 (Sept. 1965).

Another method of synthesizing nonuniformly spaced arrays, M. T. Ma, IEEE Trans. Ant. Prop. **AP–13,** No. 5, 833–834 (Sept. 1965).

On the relation between auroral radio absorption and very low frequency emissions, W. L. Ecklund, J. K. Hargreaves, and J. H. Pope, J. Geophys. Res. **70,** No. 17, 4285–4292 (Sept. 1, 1965).

The effect of ion-drag on the neutral air in the ionospheric *F*-region, H. Rishbeth and L. R. Megill, Ann. Geophys. **21,** No. 2, 235–244 (Apr.–June 1965).

Deuterium isotope effect in vacuum-ultraviolet absorption coefficients of water and methane, A. H. Laufer and J. R. McNesby, Can. J. Chem. **43,** No. 12, 3487–3490 (Dec. 1965).

Electrochemical methods, J. K. Taylor, E. J. Maienthal, and G. Marinenko, Book, Trace Analysis: Physical Methods, ed. G. H. Morrison, ch. 10, pp. 377–433 (Interscience Publ. Inc., New York, N.Y., 1965).

Interaction of oxygen with platinum, A. J. Melmed, J. Appl Phys. **36,** No. 11, 3691–3692 (Nov. 1965).

Proton transfer reactions occurring in the gas-phase radiolysis, P. Ausloos and S. G. Lias, Discussions Faraday Soc. **39,** 36–44 (1964).

Restoration of complete dentures inadvertently warped by the patient: Report of case, J. B. Woelfel and G. C. Paffenbarger, J. Am. Dental Assoc. **71,** 866–870 (Oct. 1965).

Solid-vapor equilibrium in the system hydrogen-methane, M. J. Hiza and R. N. Herring (Proc. 1965 Cryogenic Engineering Conf., Philadelphia, Pa., Aug. 17–21, 1964), Book, International Advances in Cryogenic Engineering, ed. K. D. Timmerhaus, 10, Sec. Q, pp. 182 (Plenum Press Inc., New York, N.Y., 1965).

Spectrophotometric determination of bromine and hydrogen bromide, E. C. Creitz, Anal. Chem. **37,** 1690–1692 (Dec. 1965).

Comment of obscurities of oscillator noise, L. Fey, W. R. Atkinson, and J. Newman, Proc. IEEE Letter **52,** 104–105 (Jan. 1964).

Cryogenic fluid, two-phase critical flow studies related to reactor systems, R. V. Smith, H. S. Isbin, H. K. Fauske, M. Petrick, C. H. Robbins, and F. R. Zuludek, Proc. 3d United Nations Intern. Conf. Peaceful Uses of Atomic Energy, Geneva, Switzerland, Aug. 31–Sept. 9, 1964.

Field strength calibration techniques at the NBS, H. E. Taggart, IEEE Trans. Electromag. Compatability **EC–7,** No. 2, 163–169 (June 1965).

Field-strength measurements in a multipath field, C. C. Watterson, Proc. 4th Natl. IEEE Symp. Radio Frequency Interference, San Francisco, Calif., June 28–29, 1962.

Gearing errors as related to alignment techniques of the rotary-vane attenuator, W. Larson, 19th Annual IEEE Conference and Exhibit on Instrumentation and Measurements, New York, N. Y., Oct. 12–15, 1964, Preprint No. 12–5–2–64 (Sept. 1965); IEEE Instr. Meas. **IM–14,** No. 3, 117–123 (Sept. 1965).

Optical instrumentation for the biologist, J. R. Meyer-Arendt, Appl. Opt. **4,** No. 1, 1–9 (Jan. 1965).

The NBS cryogenic data center, Proc. XI Intern. Congress Refrigeration, Munich, Germany, Aug. 28, 1963, pp. 110–114 (1965).

Timing and space navigation with an existing ground based system, G. Hefley, R. F. Linfield, and R. H. Doherty, AGARD Navigation Systems for Aircraft and Space Vehicles, pp. 490–506 (Pergamon Press Inc., New York, N. Y., 1962).

22 ISCC–NBS centroid colors of maximum contrast, K. L. Kelly, Color Engr. **3,** No. 6, 26–27 (Nov.–Dec. 1965).

A stable arc source of high ultraviolet radiance, C. R. Yokley, Proc. Symp. Solar Radiation Simulation, Los Angeles, Calif., Jan. 18–20, 1965, pp. 107–110 (1965).

A latitude survey of the night airglow, T. N. Davis and L. L. Smith, J. Geophys. Res. **70,** No. 5, 1127–1138 (Mar. 1965).

A theoretical study of the Martian and Cynytherian ionospheres, R. B. Norton, Natl. Aeronautic. Space Admin. Tech. Note TN D–2333 (1964).

Atomic lifetimes in neon I, J. Z. Klose, Phys. Rev. **141,** No. 1, 181–188 (Jan. 7, 1966).

Coherent Raman effect in the off-axis Raman resonator, D. A. Jennings and H. Takuma, Appl. Phys. Letters **4,** No. 11, 185–186 (June 1964).

Comment on the "Difference between a non-LTE, and a pure absorption, model for the line-blanketing effect," R. N. Thomas, Astrophys. J. **141,** No. 1, 333–335 (Jan. 1965).

Flare importance ratings—some hope for improvement, C. S. Warwick, Proc. Natl. Aeronautic Space Admin. Flare Conf. The Physics of Solar Flares, pp. 27–28 (1964).

Infrasonic observations of the May 16, 1964, volcanic explosion on the island of Bali, V. H. Goerke, J. M. Young, and R. K. Cook, J. Geophys. Res. **70,** No. 24, 6017–6022 (Dec. 15, 1965).

Interaction of 350-keV polarized neutrons with oriented ^{165}Ho nuclei, R. Wagner, P. D. Miller, T. Tamura, and H. Marshak, Phys. Rev. **139,** No. 1B, B29–B46 (July 12, 1965).

Nonanalyticity of transport coefficients and the complete density expansion of momentum correlation functions, J. Weinstock, Phys. Rev. **140,** No. 2A, A460–A465 (Oct. 18, 1965).

Non-linear ambipolar diffusion across a magnetic field, K. B. Persson and E. R. Mosburg, Phys. Fluids **7,** No. 11, 1829–1833 (Nov. 1964).

Nuclear size determination by neutral-pion photoproduction, R. A. Schrack, Phys. Rev. **140,** No. 4B, B987–B904 (Nov. 22, 1965).

On the use of thermopiles for absolute radiometry in the far ultraviolet, R. G. Johnston, and R. P. Madden, Appl. Opt. **4,** No. 12, 1574–1580 (Dec. 1965).

Phonon induced nuclear dipole transitions, R. J. Mahler (Proc. XIIIth Colloque and Relaxation in Solids), Book, Nuclear Magnetic Resonance and Relaxation in Solids, ed. L. V. Gerven, pp. 202–209 (North Holland Publ. Co., Amsterdam, The Netherlands, 1965).

Remarks on a paper by T. Makino "On the cosmic-ray cut-off rigidities and the earth's magnetic Field," H. H. Sauer, Report of Ionosphere and Space Research in Japan **19,** No. 1, 54–55 (1965).

Solute nuclear magnetic resonances in primary lead alloys, L. H. Bennett, R. M. Cotts, and R. J. Snodgrass (Proc. XIIIth Colloque and Relaxation in Solids), Book, Nuclear Magnetic Resonance and Relaxation in Solids, ed. L. V. Gerven, pp. 171–180 (North-Holland Publ. Co., Amsterdam, The Netherlands, 1965).

Spectra of C_2 in solidified gases at 4° and 20° K, R. L. Barger and H. P. Broida, J. Chem. Phys. **43,** No. 7, 2371–2376 (Oct. 1, 1965).

Spectra of C_3 in solidified gases at 4° and 20° K, R. L. Barger and H. P. Broida, J. Chem. Phys. **43,** No. 7, 2364–2370 (Oct. 1, 1965).

Spectrum of stationary homogeneous magnetohydrodynamic turbulence, C. M. Tchen, Phys. Fluid **8,** No. 9, 1659–1667 (Sept. 1965).

Suppression at high temperature of effects due to statistics in the second virial coefficient of a real gas, S. Y. Larsen, J. E. Kilpatrick, E. H. Keb, and H. F. Jordan, Phys. Rev. **140,** No. 1A, A129–A130 (Oct. 1965).

The brush cathode plasma—a well behaved plasma, K. B. Persson, J. Appl. Phys. **36,** No. 10, 3086 (Oct. 1965).

The realization and use of the international practical temperature scale of 1948, J. P. Evans, ISA 20th Annual Conference and Exhibit, Los Angeles, Calif., Oct. 4–7, 1965), ISA Preprint 14.3–1–65 (1965).

The relationship of a.c. resonant probes to resonant scattering, W. M. Leavens, Physics Letters **19,** No. 2, 118–120 (Oct. 1, 1965).

Thermal conductivity and viscosity of simple fluids, J. V. Sengers, Intern. J. Heat Mass Transfer **8,** 1103–1116 (1965).

A study of auroral absorption events at the south pole: 2. Conjugate properties, J. K. Hargreaves and H. J. A. Chivers, J. Geophys. Res. **70,** No. 5, 1093–1102 (Mar. 1965).

Characteristic variations in the antarctic ionosphere, V. L. Peterson, G. Stonehocker, and J. W. Wright, Antarctic Research Series, Am. Geophys. Union, Geomagnetism and Aeronomy **4**, 47–75 (1965).

International comparison on dielectric measurements, E. Rushton, G. Russell, B. W. Petley, H. E. Bussey, J. E. Gray, E. C. Bamberger, and D. Morris, IEEE Trans. Instru. Meas. **IM-13**, No. 4, 305–311 (Dec. 1964).

Interrelations of sporadic *E* and ionospheric currents, S. Matsushita, Book, Ionospheric Sporadic-*E*, ed. E. K. Smith and S. Matsushita, ch. II, pt. C, No. 5, 344–375 (Pergamon Press Inc., New York, N.Y., 1962).

Lightning characteristics as derived from sferics, W. L. Taylor (Proc. 3d Intern. Conf. Atmospheric and Space Electricity, Montreus, Switzerland, May 1963), Book, Problems of Atmospheric and Space Electricity, ed. S. C. Coroniti, pp. 388–404 (Elsevier Publ. Corp., Amsterdam, The Netherlands, 1965).

Long term characteristics for air-ground propagation in band nine, R. S. Kirby, IEEE Antenna propagation Intern. Symp. Digest, pp. 43–47 (July 9–11, 1963).

On the continuity equation for electron density in the ionosphere, T. Shimazaki, J. Atmospheric Terrest. Phys. **27**, 593–604 (1965).

Studies of Alouette observations at the CRPL, W. Calvert, H. Rishbeth, and T. Van Zandt, Trans. American Geophysical Union, IG Bull. **45**, No. 2, 398–401 (June 1964).

Topside sounding as a tool for global ionosphere studies, R. W. Knecht, IEEE Trans. Ant. Prop. Programs Digest, pp. 21–23 (1963).

Gas phase radiolysis and vacuum ultraviolet photolysis of 2- and 3-pentanone, A. Scala and P. Ausloos, J. Phys. Chem. **70**, No. 1, 260–269 (Jan. 1966).

New developments in dental materials: a world-wide survey, G. C. Paffenbarger, Intern. Dental J. **15**, No. 3, 311–422 (Sept. 1965).

Quenching of the triplet state of acetone and biacetyl by various unsaturated hydrocarbons, R. E. Rebbert and P. Ausloos, J. Am. Chem. Soc. **87**, No. 24, 5569–5572 (Dec. 20, 1965).

Vacuum-ultraviolet photolysis of ethane at high temperature. II. Collisional deactivation of excited ethylene, R. F. Hampson, Jr., and J. R. McNesby, J. Chem. Phys. **43**, No. 10, 3592–3596 (Nov. 15, 1965).

Foreword, R. G. Scott, Book, Cryogenics, pp. V (Reinhold Publ. Corp., New York, N.Y., 1964).

MAGIC-A machine for automatic graphics interface to a computer, D. E. Rippy and D. C. Humphries, Proc. Fall Joint Computer Conf., Nov. 20–Dec. 2, 1965, Las Vegas, Nevada, pp. 819–830 (Spartan Books, Inc., Wash., D.C., 1965).

The NBS time scale and its relation to other time scales, J. A. Barnes and R. C. Mockler (Proc. XIV General Assembly of URSI, Tokyo, Japan, 1963), Book, Progress in Radio Science 1960–1963. Vol. **I.** Radio Standards and Measurements, ed. R. W. Beatty, p. 41 (Elsevier Pub. Co., Amsterdam, The Netherlands, 1965).

Annual report of the National Bureau of Standards, C. E. Moore, Astron. J. **70**, No. 9, 637–639 (Nov. 1965).

Oxygen metastable atom production through photodetachment, L. M. Branscomb, S. J. Smith, and G. C. Tisone, J. Chem. Phys. **43**, No. 8, 2906–2907 (Oct. 15, 1965).

The current revision of the solar spectrum table λ2935Å to λ8770Å, C. E. Moore, Proc. Utrecht Symp. Solar Spectrum, Utrecht, The Netherland, Aug. 26–31, 1963, ed. C. DeJager, pp. 89–101 (D. Reidel Publ. Co., Dordrecht, The Netherlands, 1965).

Total cross section of 14 MeV neutrons using aligned ^{165}Ho nuclei, H. Marshak, A. Richardson, and T. Tamura, Phys. Rev. Letters **16**, No. 5, 194–197 (Jan. 31, 1966).

Influence of irregular terrain on propagation, J. W. Herbstreit (Proc. XIV General Assembly of URSI, Tokyo, Japan, 1963), Book, Progress in Radio Science 1960–1963. Vol. **II.** Radio and Troposphere, ed. F. du Castel, pp. 141–156 (Elsevier Publ. Co., Amsterdam, The Netherlands, 1965).

**Publications for which a price is indicated are available by purchase from the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C., 20402 (foreign postage, one-fourth additional). Reprints from outside journals and the NBS Journal of Research may often be obtained directly from the authors.*

U.S. GOVERNMENT PRINTING OFFICE : 1966 0L—211–570

UNIVERSITY MICROFILMS, INC.

UNI
GOVERNMEN
DIVISION OF PUBLIC DOCUMENTS
WASHINGTON, D.C. 20402

OFFICIAL BUSINESS

POSTAGE AND FEES PAID
U.S. GOVERNMENT PRINTING OFFICE

JOURNAL OF RESEARCH of the National Bureau of Standards Vol. 70B, No. 2 April–June 1966
B. Mathematics and Mathematical Physics

Contents

	Page
On a sequence of points of interest for numerical quadrature. Seymour Haber.	127
On abstract numerical integrations. John J. Sopka.	137
Treatment of outliers in samples of size three. F. J. Anscombe and Bruce A. Barron.	141
A note on contaminated samples of size three. T. A. Willke.	149
Realizing the distance matrix of a graph. A. J. Goldman.	153
Pairs of nonsingular matrices. Karl Goldberg.	155
Upper bounds for the determinant of a row stochastic matrix. Karl Goldberg.	157
Groups preserving ordering in vectors. Karl Goldberg.	159
Publications of the National Bureau of Standards.	161

Library of Congress Catalog Card Number: 62–4414

For sale by the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402. Price 75 cents (single copy). Subscription price: $2.25 a year, $0.50 additional for foreign mailing.
UNITED STATES GOVERNMENT PRINTING OFFICE, WASHINGTON : 1965